Synthesis of Functionalized Tetrahydrodibenzo[*b*,*g*] [1,8]naphthyridin-1(2*H*)-ones through Base-promoted Annulation of Quinoline Derived Dipolarophile and Cyclic Enaminones

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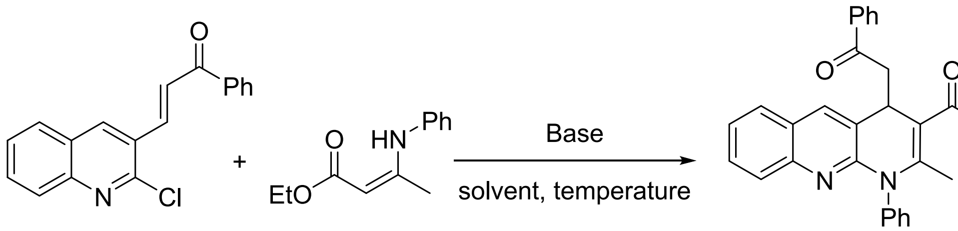
Contents

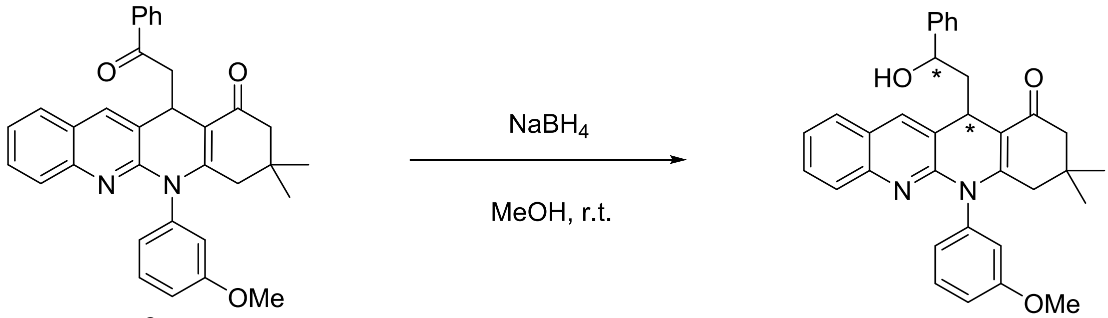
1. 3-(2-chloroquinolin-3-yl)-1-phenylprop-2-en-1-one 1a with linear enamine esters 2a' react



Entry	Base	Solvent	Temp(°C)	Yield(%)
1	Cs_2CO_3	CH_3CN	80	22
2	NaOH	CH_3CN	80	23
3	**KOH**	**CH_3CN**	**80**	**30**
4	*t*-BuOK	CH_3CN	80	23
5	NaO*t*Bu	CH_3CN	80	24
6	*t*-BuOK	CH_3CN	80	20
7	*t*-BuOK	THF	reflux	23
8	KOH	DMSO	80	20

Ethyl 2-methyl-4-(2-oxo-2-phenylethyl)-1-phenyl-1,4-dihydrobenzo[*b*][1,8]naphthyridine-3-carboxylate (3a'). 30% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.96-7.89 (m, 3H), 7.66-7.59 (m, 1H), 7.56-7.46 (m, 5H), 7.46-7.34 (m, 5H), 7.30-7.24 (m, 1H), 4.96 (dd, *J* = 8.6, 4.0 Hz, 1H), 4.24 (tdd, *J* = 10.8, 7.2, 3.6 Hz, 2H), 3.37 (qd, *J* = 15.6, 6.4 Hz, 2H), 2.22 (s, 3H), 1.32 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ 200.7, 198.0, 167.3, 151.4, 150.9, 145.8, 140.0, 137.1, 136.0, 133.0, 130.6, 129.0, 128.9, 128.5, 128.1, 128.0, 127.9, 127.0, 126.3, 124.1, 122.0, 102.6, 60.0, 47.0, 34.7, 19.4, 14.4. HRMS (ESI) m/z calculated for $C_{30}H_{27}N_2O_3$ $[M+H]^+$ = 463.2016, found = 463.2018.

2. Transformations of the product 3q



3q **4/4'** 92% yield, d.r. = 1:1

To a 50-mL flame-dried flask was charged with **3q** (150.6 mg, 0.3 mmol) in MeOH (5 mL) was added $NaBH_4$ (22.6 mg, 0.6 mmol). The reaction mixture was stirred for 1.0 h at room temperature, and the solvent saturated aq. $NaHCO_3$ (3 mL) was added. The phases were separated and the aqueous layer was extracted with DCM (3 x 2 mL). The combined organic extracts, dried over Na_2SO_4, filtered, and concentrated in vacuo. The crude residue was purified by flash column chromatography (PE: EA = 5:1) on silica gel to give the compound **4** (70mg, 46% yield) and **4'** (69mg, 46% yield).

12-(2-hydroxy-2-phenylethyl)-5-(3-methoxyphenyl)-3,3-dimethyl-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (4)

Yellow foam solid, m.p.: 72-73 °C, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.93 (s, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.60 (d, J = 8.4 Hz, 1H), 7.52-7.43 (m, 2H), 7.39-7.27 (m, 5H), 7.20 (t, J = 7.2 Hz, 1H), 7.10-7.05 (m, 1H), 6.88 (d, J = 8.8 Hz, 2H), 4.66 (dd, J = 11.6, 3.6 Hz, 1H), 4.62-4.56 (m, 1H), 3.89 (s, 3H), 2.48-2.34 (m, 2H), 2.24 (q, J = 17.6 Hz, 2H), 2.07-1.95 (m, 1H), 1.92-1.79 (m, 2H), 1.15 (s, 3H), 1.05 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ 197.6, 160.4, 156.0, 150.3, 145.5, 143.8, 140.0, 135.5, 129.9, 129.0, 128.2, 126.9, 126.8, 126.8, 125.7, 124.8, 124.1, 113.8, 110.6, 69.5, 55.5, 51.6, 49.9, 42.5, 32.1, 31.2, 29.9, 26.6. HRMS (ESI) m/z calculated for $C_{33}H_{33}N_2O_3$ $[M+H]^+$ = 505.2486, found = 505.2486.

12-(2-hydroxy-2-phenylethyl)-5-(3-methoxyphenyl)-3,3-dimethyl-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (4')

Yellow foam solid, m.p.: 75-76 °C, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.11 (s, 1H), 7.75 (d, *J* = 7.2 Hz, 1H), 7.62 (d, *J* = 8.4 Hz, 1H), 7.54-7.48 (m, 1H), 7.45 (t, *J* = 8.0 Hz, 1H), 7.39-7.33 (m, 1H), 7.29-7.26 (m, 3H), 7.22-7.16 (m, 1H), 7.08-7.02 (m, 1H), 6.86 (dd, *J* = 8.0, 4.8 Hz, 2H), 4.76 (dd, *J* = 10.0, 3.2 Hz, 1H), 4.69 (dd, *J* = 8.4, 4.0 Hz, 1H), 3.87 (s, 3H), 2.25 (q, *J* = 16.4 Hz, 2H), 2.18-2.01 (m, 3H), 1.95 (ddd, *J* = 14.0, 8.8, 3.6 Hz, 1H), 0.98 (s, 6H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ 195.9, 160.4, 154.4, 150.4, 145.7, 144.9, 140.2, 136.1, 129.8, 129.0, 128.3, 128.2, 127.1, 126.6, 125.7, 124.6, 123.0, 113.9, 111.7, 71.0, 55.5, 50.1, 48.2, 42.1, 32.6, 31.2, 29.1, 27.3. HRMS (ESI) m/z calculated for $C_{33}H_{33}N_2O_3$ $[M+H]^+$ = 505.2486, found = 505.2489.

3. Characterization of 3

5-(4-methoxyphenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3a). 96% yield, red oily, ^{1}**H NMR** (400 MHz, $CDCl_3$): δ 8.02-7.96 (m, 2H), 7.83 (s, 1H), 7.64-7.47 (m, 4H), 7.45-7.38 (m, 3H), 7.30-7.26 (m, 2H), 7.06 (d, *J* = 8.8 Hz, 2H), 4.96 (dd, *J* = 7.6, 3.6 Hz, 1H), 3.91 (s, 3H), 3.56-3.29 (m, 2H), 2.34-2.21 (m, 2H), 2.16-2.02 (m, 2H), 0.99 (s, 3H), 0.98 (s, 3H). ^{13}**C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.2, 195.4, 159.0, 155.4, 151.0, 145.7, 137.0, 136.2, 132.8, 132.0, 131.1, 128.9, 128.5, 128.2, 128.1, 126.8, 124.4, 122.3, 114.4, 109.7, 55.4, 50.0, 46.6, 42.4, 32.5, 31.7, 29.1, 27.3. HRMS (ESI) m/z calculated for $C_{33}H_{31}N_2O_3$ $[M+H]^+$ = 503.2329, found = 503.2330.

3,3-dimethyl-12-(2-oxo-2-phenylethyl)-5-phenyl-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3b). 75% yield, red oily,^{1}**H NMR** (400 MHz, $CDCl_3$): δ 8.03-7.96 (m, 2H), 7.85 (s, 1H), 7.62-7.47 (m, 6H), 7.62-7.48 (m, 5H), 7.29-7.26 (m, 1H), 4.98 (dd, *J* = 7.6, 3.6 Hz, 1H), 3.56-3.33 (m, 2H), 2.35-2.22 (m, 2H), 2.18-2.00 (m, 2H), 0.99 (s, 3H), 0.98 (s, 3H). ^{13}**C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.1, 195.4, 154.83, 150.8, 145.6, 139.4, 137.0, 136.2, 132.8, 130.3, 129.2, 128.9, 128.5, 128.2, 128.1, 128.0, 126.8, 126.3, 124.5, 122.2, 109.7, 50.1, 46.6, 42.3, 32.5, 31.7, 29.1, 27.2. HRMS (ESI) m/z calculated for $C_{32}H_{29}N_2O_2$ $[M+H]^+$ = 473.2224, found = 473.2232.

3,3-dimethyl-12-(2-oxo-2-phenylethyl)-5-(p-tolyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3c). 96% yield, red oily, ^{1}**H NMR** (400 MHz, $CDCl_3$): δ 8.00 (d, *J* = 7.2 Hz, 2H), 7.83 (s, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.56-7.48 (m, 2H), 7.47-7.40 (m, 3H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.26-7.22 (m, 3H), 4.97 (dd, *J* = 7.2, 3.6 Hz, 1H), 3.50-3.31 (m, 2H), 2.50 (s, 3H), 2.33-2.22 (m, 2H), 2.17-2.03 (m, 2H), 0.99 (s, 3H), 0.98 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.2, 195.3, 155.1, 150.9, 145.6, 137.9, 137.0, 136.7, 136.2, 132.8, 129.9, 128.9, 128.5, 128.3, 128.0, 126.8, 126.3, 124.4, 122.2, 109.7, 50.1, 46.6, 42.3, 32.5, 31.7, 29.1, 27.3, 21.3. HRMS (ESI) m/z calculated for $C_{33}H_{31}N_2O_2$ $[M+H]^+$ = 487.2381, found = 487.2388.

5-(4-ethylphenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3d). 82% yield, red oily,**^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.04-7.97 (m, 2H), 7.83 (s, 1H), 7.62-7.48 (m, 3H), 7.46-7.35 (m, 5H), 7.29-7.25 (m, 3H), 4.98 (dd, *J* = 7.6, 3.6 Hz, 1H), 3.52-3.31 (m, 2H), 2.80 (q, *J* = 7.6 Hz, 2H), 2.35-2.21 (m, 2H), 2.18-2.01 (m, 2H), 1.37 (t, *J* = 7.6 Hz, 3H), 0.99 (s, 6H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.2, 195.4, 155.2, 150.9, 145.7, 144.1, 137.0, 136.8, 136.3, 132.9, 129.9, 128.9, 128.6, 128.5, 128.3, 128.1, 126.8, 126.3, 124.4, 122.3, 109.8, 50.2, 46.7, 42.3, 32.5, 31.8, 29.1, 28.5, 27.3, 15.2. HRMS (ESI) m/z calculated for $C_{34}H_{33}N_2O_2$ $[M+H]^+$ = 501.2537, found = 501.2546.

5-(4-isopropylphenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3e). 95% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.03-7.97 (m, 2H), 7.83 (s, 1H), 7.62-7.48 (m, 3H), 7.46-7.37 (m, 5H), 7.28-7.26 (m, 3H), 4.98 (dd, *J* = 7.6, 3.6 Hz, 1H), 3.52-3.31 (m, 2H), 3.05 (dt, *J* = 13.6, 6.8 Hz, 1H), 2.36-2.21 (m, 2H), 2.16-2.00 (m, 2H), 1.37 (d, *J* = 6.8 Hz, 6H), 0.99 (s, 6H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.2, 195.4, 155.2, 150.9, 148.7, 145.7, 137.0, 136.9, 136.2, 132.9, 129.9, 128.9, 128.5, 128.3, 128.1, 127.2, 126.8, 126.3, 124.4, 122.3, 109.8, 50.2, 46.6, 42.3, 33.8, 32.5, 31.8, 29.1, 27.4, 24.0, 23.9. HRMS (ESI) m/z calculated for $C_{35}H_{35}N_2O_2$ $[M+H]^+$ = 515.2694, found = 515.2698.

5-(4-(tert-butyl)phenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3f). 72% yield, red oily, **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.04-7.95 (m, 2H), 7.83 (s, 1H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.55 (d, *J* = 8.4 Hz, 3H), 7.53-7.49 (m, 1H), 7.45-7.40 (m, 3H), 7.30-7.26 (m, 3H), 4.98 (dd, *J* = 7.8, 3.6 Hz, 1H), 3.49-3.30 (m, 2H), 2.34-2.22 (m, 2H), 2.18-2.03 (m, 2H), 1.44 (s, 9H), 1.00 (s, 6H). **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$): δ 198.2, 195.4, 155.2, 151.02, 150.96, 145.7, 137.1, 136.6, 136.3, 132.9, 129.6, 128.9, 128.5, 128.3, 128.2, 126.8, 126.3, 126.1, 124.5, 122.3, 109.8, 50.2, 46.7, 42.4, 34.8, 32.6, 31.8, 31.4, 29.1, 27.4. HRMS (ESI) m/z calculated for $C_{36}H_{37}N_2O_2$ $[M+H]^+$ = 529.2850, found = 529.2863.

5-([1,1'-biphenyl]-4-yl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3g). 87% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.04-7.97 (m, 2H), 7.86 (s, 1H), 7.80 (d, *J* = 8.4 Hz, 2H), 7.76-7.71 (m, 2H), 7.66-7.55 (m, 2H), 7.54-7.49 (m, 3H), 7.48-7.38 (m, 6H), 7.31-7.26 (m, 1H), 5.00 (dd, *J* = 7.6, 3.6 Hz, 1H), 3.59-3.35 (m, 2H), 2.38-2.24 (m, 2H), 2.23-2.10 (m, 2H), 1.02 (s, 3H), 1.01 (s, 3H). **^{113}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.2, 195.4, 154.9, 150.9, 145.7, 140.9, 140.2, 138.6, 137.0, 136.3, 132.9, 130.6, 129.0, 128.9, 128.5, 128.3, 128.1, 127.9, 127.7, 127.1, 126.9, 126.4, 124.5, 122.3, 110.0, 50.2, 46.7, 42.5, 32.6, 31.8, 29.1, 27.4. HRMS (ESI) m/z calculated for $C_{38}H_{33}N_2O_2$ $[M+H]^+$ = 549.2537, found = 549.2538.

3,3-dimethyl-5-(4-(methylthio)phenyl)-12-(2-oxo-2-phenylethyl)-3,4,5,12-

tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3h). 96% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.01-7.95 (m, 2H), 7.83 (s, 1H), 7.63-7.48 (m, 3H), 7.47-7.38 (m, 5H), 7.33-7.27 (m, 3H), 4.96 (dd, *J* = 7.2, 3.6 Hz, 1H), 3.58-3.28 (m, 2H), 2.59 (s, 3H), 2.35-2.21 (m, 2H), 2.16-2.02 (m, 2H), 0.99 (s, 3H), 0.98 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.2, 195.4, 154.9, 150.9, 145.7, 138.7, 137.0, 136.3, 136.2, 132.9, 130.6, 129.0, 128.5, 128.3, 128.1, 126.8, 126.7, 126.3, 124.5, 122.3, 109.9, 50.1, 46.6, 42.4, 32.5, 31.7, 29.1, 27.4, 15.5. HRMS (ESI) m/z calculated for $C_{33}H_{31}N_2O_2S$ $[M+H]^+$ = 519.2101, found = 519.2101.

3,3-dimethyl-12-(2-oxo-2-phenylethyl)-5-(4-phenoxyphenyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3i). 94% yield, red oily, **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.01-7.96 (m, 2H), 7.84 (s, 1H), 7.64-7.58 (m, 2H), 7.53-7.49 (m, 1H), 7.48-7.40 (m, 5H), 7.34 (d, *J* = 8.4 Hz, 2H), 7.31-7.27 (m, 1H), 7.22 - 7.15 (m, 5H), 4.97 (dd, *J* = 7.8, 3.6 Hz, 1H), 3.55-3.33 (m, 2H), 2.35-2.24 (m, 2H), 2.20-2.09 (m, 2H), 1.02 (s, 3H), 1.00 (s, 3H). **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$): δ 198.2, 195.4, 157.1, 156.5, 155.0, 151.0, 145.7, 137.0, 136.2, 134.2, 132.9, 131.6, 129.9, 129.0, 128.5, 128.3, 128.1, 126.9, 126.4, 124.5, 123.9, 122.4, 119.6, 118.8, 109.9, 50.2, 46.6, 42.5, 32.6, 31.7, 29.1, 27.4. HRMS (ESI) m/z calculated for $C_{38}H_{33}N_2O_2$ $[M+H]^+$ = 565.2486, found = 565.2495.

5-(4-fluorophenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3j). 88% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.00-7.93 (m, 2H), 7.84 (s, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.57-7.48 (m, 2H), 7.47-7.36 (m, 5H), 7.30-7.23 (m, 3H), 4.94 (dd, *J* = 6.8, 3.6 Hz, 1H), 3.63-3.31 (m, 2H), 2.35-2.21 (m, 2H), 2.16-2.00 (m, 2H), 1.00 (s, 3H), 0.97 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.2, 195.4, 162.1 (d, $J_{C\text{-}F}$ = 246.0 Hz), 154.8, 150.9, 145.6, 137.0, 136.2, 135.4 (d, $J_{C\text{-}F}$ = 3.0 Hz), 132.9, 132.0 (d, $J_{C\text{-}F}$ = 6.0 Hz), 129.0, 128.5, 128.2, 128.0, 126.8, 126.3, 124.6, 122.4, 116.2 (d, $J_{C\text{-}F}$ = 22.0 Hz), 109.9, 50.1, 46.6, 42.4, 32.5, 31.7, 29.1, 27.3. **^{19}F NMR** (377 MHz, $CDCl_3$): δ -113.11 – -113.21 (m). HRMS (ESI) m/z calculated for $C_{32}H_{28}FN_2O_2$ $[M+H]^+$ = 491.2130, found = 491.2140.

5-(4-chlorophenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3k). 95% yield, red oily, **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.96 (d, *J* = 7.4 Hz, 2H), 7.85 (s, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.54 (d, *J* = 8.4 Hz, 3H), 7.52-7.48 (m, 1H), 7.47-7.39 (m, 3H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.31-7.27 (m, 1H), 4.94 (dd, *J* = 7.2, 3.6 Hz, 1H), 3.60-3.32 (m, 2H), 2.35-2.22 (m, 2H), 2.16-2.02 (m, 2H), 1.00 (s, 3H), 0.98 (s, 3H). **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$): δ 198.1, 195.4, 154.4, 150.8, 145.6, 138.1, 137.0, 136.2, 134.0, 132.9, 131.8, 129.5, 129.1, 128.5, 128.2, 128.0, 126.8, 126.4, 124.6, 122.3, 110.0, 50.1, 46.6, 42.4, 32.6, 31.6, 29.1, 27.3. HRMS (ESI) m/z calculated for $C_{32}H_{28}N_2O_2$ $[M+H]^+$ = 507.1834, found = 507.1847.

5-(4-bromophenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3l). 94% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.99-7.93 (m, 2H), 7.84 (s, 1H), 7.69 (d, *J* = 8.6 Hz, 2H), 7.63-7.58 (m, 1H), 7.57-7.38 (m, 5H), 7.32-7.26 (m, 3H), 4.94 (dd, *J* = 7.2, 3.6 Hz, 1H), 3.61-3.29 (m, 2H), 2.34-2.21 (m, 2H), 2.14-2.01 (m, 2H), 1.00 (s, 3H), 0.97 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.1, 195.4, 154.3, 150.7, 145.5, 138.6, 136.9, 136.2, 132.9, 132.5, 132.1, 129.1, 128.5, 128.2, 128.0, 126.8, 126.3, 124.6, 122.3, 122.1, 110.0, 50.1, 46.5, 42.4, 32.5, 31.6, 29.1, 27.3. HRMS (ESI) m/z calculated for $C_{32}H_{28}BrN_2O_2$ $[M+H]^+$ = 551.1329, found = 551.1336.

5-(4-iodophenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3m). 91% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.97-7.93 (m, 2H), 7.89 (d, *J* = 8.8 Hz, 2H), 7.84 (s, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.55-7.48 (m, 2H), 7.46-7.38 (m, 3H), 7.31-7.26 (m, 1H), 7.15 (d, *J* = 8.4 Hz, 2H), 4.94 (dd, *J* = 7.2, 3.6 Hz, 1H), 3.58-3.32 (m, 2H), 2.33-2.22 (m, 2H), 2.14-2.02 (m, 2H), 1.00 (s, 3H), 0.97 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.2, 195.4, 154.3, 150.7, 145.6, 139.3, 138.5, 137.0, 136.2, 132.9, 132.4, 129.1, 128.5, 128.2, 128.0, 126.9, 126.4, 124.7, 122.3, 110.1, 93.7, 50.1, 46.6, 42.5, 32.6, 31.6, 29.1, 27.4. HRMS (ESI) m/z calculated for $C_{32}H_{28}IN_2O_2$ $[M+H]^+$ = 599.1190, found = 599.1192.

3,3-dimethyl-12-(2-oxo-2-phenylethyl)-5-(4-(trifluoromethyl)phenyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3n). 76% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.96 (d, *J* = 7.2 Hz, 2H), 7.87 (s, 1H), 7.86-7.81 (m, 3H), 7.65-7.49 (m, 5H), 7.48-7.38 (m, 3H), 7.34-7.27 (m, 1H), 4.95 (dd, *J* = 6.4, 3.6 Hz, 1H), 3.66-3.33 (m, 2H), 2.36-2.23 (m, 2H), 2.13-1.97 (m, 2H), 1.00 (s, 3H), 0.97 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.2, 195.5, 154.0, 150.7, 145.5, 142.9, 137.0, 136.3, 133.0, 131.1, 130.1, 129.2, 128.5, 128.2, 128.0, 126.9, 126.4 (q, $J_{C\text{-}F}$ = 7.0 Hz, $J_{C\text{-}F}$ = 3.0 Hz), 124.8, 122.3, 110.2, 50.2, 46.6, 42.5, 32.7, 31.6, 29.1, 27.4. **^{19}F NMR** (377 MHz, $CDCl_3$): δ -62.32. HRMS (ESI) m/z calculated for

$C_{33}H_{28}F_3N_2O_2$ $[M+H]^+$ = 541.2097, found = 541.2099.

3,3-dimethyl-5-(4-nitrophenyl)-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3o). 88% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.44 (d, *J* = 8.9 Hz, 2H), 7.97-7.91 (m, 2H), 7.88 (s, 1H), 7.69-7.61 (m, 3H), 7.54-7.38 (m, 5H), 7.34-7.28 (m, 1H), 4.92 (dd, *J* = 6.0, 4.0 Hz, 1H), 3.75-3.29 (m, 2H), 2.36-2.23 (m, 2H), 2.14-1.96 (m, 2H), 1.00 (s, 3H), 0.96 (s, 3H). **$^{13}C\{^1H\}$ NMR** (100 MHz, $CDCl_3$): δ 198.2, 195.5, 153.5, 150.6, 147.4, 145.7, 145.4, 136.9, 136.3, 133.0, 131.8, 129.3, 128.6, 128.1, 127.9, 126.9, 126.44, 124.9, 124.6, 122.3, 110.6, 50.1, 46.5, 42.6, 32.7, 31.5, 29.1, 27.4. HRMS (ESI) m/z calculated for $C_{32}H_{28}N_3O_4$ $[M+H]^+$ = 518.2075, found = 518.2084.

3,3-dimethyl-12-(2-oxo-2-phenylethyl)-5-(m-tolyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3p). 96% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.04-7.98 (m, 2H), 7.83 (s, 1H), 7.60 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.57-7.49 (m, 2H), 7.48-7.41 (m, 4H), 7.33-7.27 (m, 2H), 7.17 (d, *J* = 1.2 Hz, 2H), 4.98 (dd, *J* = 7.6, 4.0 Hz, 1H), 3.51-3.32 (m, 2H), 2.47 (s, 3H), 2.34-2.22 (m, 2H), 2.17-2.03 (m, 2H), 0.99 (s, 3H), 0.99 (s, 3H). **$^{13}C\{^1H\}$ NMR** (100 MHz, $CDCl_3$): δ 198.2, 195.4, 155.0, 150.9, 145.7, 139.3, 139.2, 137.0, 136.2, 132.9, 128.9, 128.5, 128.3, 128.1, 126.9, 126.3, 124.5, 122.2, 109.7, 50.2, 46.7, 42.4, 32.6, 31.8, 29.1, 27.4, 21.4. HRMS (ESI) m/z calculated for $C_{33}H_{31}N_2O_2$ $[M+H]^+$ = 487.2380, found = 487.2396.

5-(3-methoxyphenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3q). 91% yield, red oily, **^{1}H**

NMR (400 MHz, $CDCl_3$): δ 8.02-7.94 (m, 2H), 7.84 (s, 1H), 7.63-7.54 (m, 2H), 7.52-7.38 (m, 5H), 7.30-7.24 (m, 1H), 7.07-7.02 (m, 1H), 7.00-6.94 (m, 2H), 4.97 (dd, *J* = 7.6, 3.6 Hz, 1H), 3.87 (s, 3H), 3.55-3.32 (m, 2H), 2.36-2.22 (m, 2H), 2.20-2.07 (m, 2H), 0.99 (d, *J* = 3.3 Hz, 6H). **$^{13}C\{^1H\}$ NMR** (100 MHz, $CDCl_3$): δ 198.1, 195.3, 160.3, 154.8, 150.7, 145.6, 140.5, 136.9, 136.1, 132.8, 129.7, 128.8, 128.4, 128.2, 128.0, 126.8, 126.3, 124.4, 122.2, 113.8, 109.7, 55.4, 50.1, 46.6, 42.1, 32.5, 31.7, 29.1, 27.2. HRMS (ESI) m/z calculated for $C_{33}H_{31}N_2O_3$ $[M+H]^+$ = 503.2329, foun = 503.233d3.

5-(3-fluorophenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3r). 90% yield, red oily, **^1H NMR** (400 MHz, $CDCl_3$): δ 7.96 (d, *J* = 8.0 Hz, 2H), 7.85 (s, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.55-7.48 (m, 3H), 7.47-7.39 (m, 3H), 7.32-7.24 (m, 2H), 7.22-7.17 (m, 2H), 4.97-4.91 (m, 1H), 3.61-3.31 (m, 2H), 2.33-2.22 (m, 2H), 2.17-2.03 (m, 2H), 1.00 (s, 3H), 0.98 (s, 3H). **$^{13}C\{^1H\}$ NMR** (100 MHz, $CDCl_3$): δ 198.1, 195.5, 163.1 (d, J_{C-F} = 246.0 Hz), 154.4, 150.7, 145.6, 141.0 (d, J_{C-F} = 10.0 Hz), 137.0, 136.2, 132.9 , 130.2 (d, J_{C-F} = 9.0 Hz), 129.1, 128.5, 128.2, 128.1, 126.9, 126.4, 126.3 (d, J_{C-F} = 2.0 Hz), 124.7, 122.3, 118.1 (d, J_{C-F} = 22.0 Hz), 115.5 (d, J_{C-F} = 20.0), 110.0, 50.2, 46.6, 42.3, 32.6, 31.6, 29.1, 27.3. **^{19}F NMR** (377 MHz, $CDCl_3$): δ -111.3 – -111.69 (m). HRMS (ESI) m/z calculated for $C_{32}H_{28}FN_2O_2$ $[M+H]^+$ = 491.2129, found = 491.2142.

5-(3-chlorophenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3s). 96% yield, red oily, **^1H NMR** (400 MHz, $CDCl_3$): δ 8.00-7.93 (m, 2H), 7.86 (s, 1H), 7.64-7.59 (m, 1H), 7.57-7.52 (m, 1H), 7.52-7.39 (m, 7H), 7.34-7.27 (m, 2H), 4.94 (dd, *J* = 7.2, 3.6 Hz, 1H), 3.62-3.30 (m, 2H), 2.35-2.22 (m, 2H), 2.17-2.00 (m, 2H), 1.01 (s, 3H), 0.98 (s, 3H).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 198.1, 195.5, 154.3, 150.7, 145.6, 143.0, 140.7, 136.7, 136.3, 134.7, 133.0, 130.7, 130.1, 129.1, 128.5, 128.2, 128.1, 128.0, 126.9, 126.4, 124.7, 122.3, 110.1, 50.2, 46.6, 42.4, 32.6, 31.6, 29.1, 27.4. HRMS (ESI) m/z calculated for $C_{32}H_{28}ClN_2O_2$ $[M+H]^+$ = 507.1834, found = 507.1836.

5-(3-bromophenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3t). 91% yield, red oily, **^1H NMR** (600 MHz, $CDCl_3$): δ 8.00-7.93 (m, 2H), 7.86 (s, 1H), 7.66-7.60 (m, 2H), 7.60-7.58 (m, 1H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.52-7.49 (m, 1H), 7.47-7.39 (m, 4H), 7.37 (d, *J* = 7.8 Hz, 1H), 7.31-7.27 (m, 1H), 4.95 (dd, *J* = 7.2, 3.6 Hz, 1H), 3.59-3.33 (m, 2H), 2.33-2.24 (m, 2H), 2.15-2.03 (m, 2H), 1.01 (s, 3H), 0.99 (s, 3H). **$^{13}C\{^1H\}$ NMR** (150 MHz, $CDCl_3$): δ 198.1, 195.4, 154.2, 150.6, 145.5, 140.8, 136.9, 136.3, 133.5, 132.9, 131.4, 130.4, 129.4, 129.1, 128.5, 128.2, 128.1, 126.9, 126.4, 124.7, 122.5, 122.2, 110.1, 50.1, 46.6, 42.4, 32.6, 31.59, 29.1, 27.4. HRMS (ESI) m/z calculated for $C_{32}H_{28}BrN_2O_2$ $[M+H]^+$ = 551.1329, found = 551.1329.

5-(3-iodophenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3u). 95% yield, red oily, **^1H NMR** (600 MHz, $CDCl_3$): δ 7.99-7.94 (m, 2H), 7.86 (s, 1H), 7.84 (d, *J* = 7.8 Hz, 1H), 7.79-7.74 (M, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.53-7.49 (M, 1H), 7.47-7.44 (m, 1H), 7.43-7.37 (m, 3H), 7.32-7.27 (m, 2H), 4.94 (dd, *J* = 7.2, 3.6 Hz, 1H), 3.59-3.29 (m, 2H), 2.35-2.22 (m, 2H), 2.14-2.01 (m, 2H), 1.00 (s, 3H), 0.99 (s, 3H). **$^{13}C\{^1H\}$ NMR** (150 MHz, $CDCl_3$): δ 198.1, 195.4, 154.3, 150.6, 145.5, 140.6, 139.1, 137.3, 136.9, 136.3, 132.9, 130.6, 130.0, 129.1, 128.5, 128.2, 128.1, 126.9, 126.4, 124.7, 122.2, 110.1, 93.8, 50.1, 46.6, 42.4, 32.6, 31.6, 29.0, 27.4. HRMS (ESI) m/z calculated for $C_{32}H_{28}IN_2O_2$ $[M+H]^+$ = 599.1190, found = 599.1205.

5-(benzo[d][1,3]dioxol-5-yl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3v). 89% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.01-7.94 (m, 2H), 7.83 (s, 1H), 7.65-7.57 (m, 2H), 7.53-7.39 (m, 4H), 7.31-7.27 (m, 1H), 6.96 (d, *J* = 8.2 Hz, 1H), 6.91-6.82 (m, 2H), 6.11 (dd, *J* = 7.2, 1.2 Hz, 2H), 4.94 (dd, *J* = 7.3, 3.6 Hz, 1H), 3.55-3.30 (m, 2H), 2.35-2.22 (m, 2H), 2.22-2.10 (m, 2H), 1.01 (s, 3H), 0.99 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.1, 195.4, 155.2, 151.0, 147.3, 145.7, 137.0, 136.2, 133.1, 132.9, 129.0, 128.5, 128.2, 128.1, 126.8, 126.3, 124.5, 122.4, 109.8, 108.3f, 101.7, 50.1, 46.6, 42.2, 32.5, 31.7, 29.2, 27.3. HRMS (ESI) m/z calculated for $C_{33}H_{29}N_2O_4$ $[M+H]^+$ = 517.2122, found = 517.2129.

5-(2-methoxyphenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3w). 96% yield, red oily, d.r. = 1:1, **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.08-7.99 (m, 2H), 7.84-7.81 (m, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.56-7.47 (m, 3H), 7.46-7.35 (m, 4H), 7.28-7.26 (m, 1H), 7.17-7.13 (m, 1H), 7.10-7.06 (m, 1H), 5.07-4.97 (m, 1H), 3.77 (d, *J* = 82.0 Hz, 3H), 3.55-3.29 (m, 2H), 2.34-2.23 (m, 2H), 2.23-1.99 (m, 2H), 1.06-0.97 (m, 6H). **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$): δ 198.35, 198.32, 195.4, 195.2, 156.8, 155.7, 155.5, 155.2, 150.4, 150.1, 145.9, 145.7, 137.2, 137.1, 136.8, 136.1, 133.1, 132.85, 132.81, 130.6, 129.9, 129.6, 128.9, 128.7, 128.6, 128.54, 128.52, 128.4, 128.3, 128.1, 128.0, 127.3, 127.1, 126.9, 126.4, 126.4, 124.3, 124.2, 122.2, 122.1, 121.4, 120.4, 112.2, 111.8, 110.7, 109.4, 55.9, 55.7, 50.2, 46.6, 46.4, 41.7, 40.9, 32.4, 31.9, 31.8, 29.6, 28.9, 27.8, 27.0.

HRMS (ESI) m/z calculated for $C_{33}H_{31}N_2O_3$ $[M+H]^+$ = 503.2329, found = 503.2342.

5-(2-fluorophenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3x). 95% yield, red oily, d.r. = 1:1, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.04-7.97 (m, 2H), 7.96-7.82 (m, 1H), 7.66-7.59 (m, 1H), 7.57-7.40 (m, 7H), 7.39-7.27 (m, 3H), 5.12-4.94(m, 1H), 3.61-3.25 (m, 2H), 2.41-2.03 (m, 4H), 1.10-0.92 (m, 6H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.3, 198.1, 195.6, 195.3, 159.9 (d, J_{C-F} = 249.0 Hz), 159.9 (d, J_{C-F} = 247.0 Hz), 154.7, 153.9, 150.2, 149.8, 145.8, 145.6, 137.2, 137.1, 136.3, 133.5, 133.0, 132.9, 131.4, 130.5 (d, J_{C-F} = 8.0 Hz), 130.2 (d, J_{C-F} = 8.0 Hz), 129.2, 129.1, 128.6, 128.4, 128.3, 128.2, 128.0, 127.4 (d, J_{C-F} = 14.0 Hz), 127.3, 127.2, 127.0, 126.6, 125.2 (d, J_{C-F} = 4.0 Hz), 124.7, 124.6, 124.2 (d, J_{C-F} = 4.0 Hz), 122.15, 122.07, 116.7 (d, J_{C-F} = 20.0 Hz), 116.3 (d, J_{C-F} = 20.0 Hz), 111.3, 110.1, 50.2, 46.5, 46.3, 41.9, 41.3, 32.6, 32.5, 31.8, 31.2, 29.7, 29.4, 29.0, 27.5, 27.2. **^{19}F NMR** (377 MHz, $CDCl_3$): δ -118.98 – -119.20 (m), -121.95 – -122.13 (m). HRMS (ESI) m/z calculated for $C_{32}H_{28}FN_2O_2$ $[M+H]^+$ = 491.2129, found = 491.2138.

5-(2,5-dimethylphenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3y). 89% yield, red oily, d.r. = 1:1, **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.09-7.98 (m, 2H), 7.86-7.80 (m, 1H), 7.62-7.58 (m, 1H), 7.56-7.49 (m, 2H), 7.48-7.45 (m, 1H), 7.44-7.41 (m, 2H), 7.28-7.26 (m, 1H), 7.23 (d, J = 7.4 Hz, 1H), 7.20-7.00 (m, 2H), 5.07-4.97 (m, 1H), 3.53-3.25 (m, 2H), 2.46 (s, 3H), 2.35-2.10 (m, 5H), 2.01 (s, 2H), 1.91-1.84 (m, 1H), 1.04-0.98 (m, 6H). **^{13}C{^{1}H}NMR** (150 MHz, $CDCl_3$): δ 198.2, 198.0, 195.3, 195.2, 155.1, 154.6, 150.03, 149.98, 146.1, 145.9, 138.3 138.2, 137.7, 137.1, 136.9, 136.5, 136.3, 136.2, 136.1, 135.5, 132.94, 132.86, 131.7, 131.5, 130.5, 128.9, 128.8, 128.7, 128.6, 128.5, 128.4, 128.3, 128.2, 128.1, 128.0, 127.4, 127.0, 126.9, 126.4, 126.3, 124.44, 124.39, 122.2, 122.0, 109.9, 109.5, 50.22, 50.15, 47.3, 46.8, 42.3, 41.5, 32.6, 32.3, 31.9, 31.8, 30.0, 28.5, 28.2, 26.6, 21.3, 18.0, 17.9. HRMS (ESI) m/z calculated for $C_{34}H_{33}N_2O_2$ $[M+H]^+$ = 501.2537, found = 501.2550.

3,3-dimethyl-5-(naphthalen-1-yl)-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3z). 92% yield, red oily, d.r. = 1:1, **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.32-8.10 (m, 1H), 8.06 -7.97 (m, 3H), 7.92-7.85 (m, 1H), 7.71-7.65 (m, 1H), 7.64-7.28 (m, 9H), 7.26-7.20 (m, 2H), 5.17-5.03 (m, 1H), 3.75-3.40 (m, 2H), 2.34-2.23 (m, 2H), 2.13-1.76 (m, 2H), 0.90 (d, J = 1.8 Hz, 3H), 0.87 (s, 3H). **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$): δ 198.3, 198.2, 195.6, 195.5, 155.5, 155.3, 151.0, 150.7, 145.8, 145.7, 137.1, 137.0, 137.0, 136.2, 136.1, 135.7, 134.5, 134.2, 133.0, 132.9, 132.3, 132.0, 129.0, 128.9, 128.8, 128.71, 128.66, 128.6, 128.53, 128.46, 128.43, 128.41, 128.3, 128.2, 128.1, 127.4, 127.2, 126.9, 126.79, 126.77, 126.5, 126.38, 126.35, 126.3, 126.0, 125.4, 124.5, 124.4, 123.4, 122.6, 122.2, 122.1, 109.9, 109.6, 50.3, 50.2, 47.2, 46.9, 42.1, 41.0, 32.5, 32.2, 32.0, 31.9, 29.7, 28.3, 27.8, 26.2. HRMS (ESI) m/z calculated for $C_{36}H_{31}N_2O_2$ $[M+H]^+$ = 523.2380, found = 523.2398.

5-(4-methoxyphenyl)-4,4-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3aa). 90% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.02-7.95 (m, 2H), 7.83 (s, 1H), 7.63-7.49 (m, 3H), 7.47-

7.40 (m, 3H), 7.29-7.25 (m, 3H), 7.05 (d, J = 9.2 Hz, 2H), 4.96 (dd, J = 7.6, 4.0 Hz, 1H), 3.91 (s, 3H), 3.49-3.15 (m, 2H), 2.31-2.07 (m, 2H), 1.69-1.65 (m, 2H), 1.13 (s, 3H), 1.10 (s, 3H). **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$): δ 200.6, 198.4, 159.1, 155.0, 150.9, 145.8, 137.2, 136.3, 132.9, 132.0 131.2, 128.9, 128.5, 128.4, 128.1, 126.9, 126.4, 124.4, 122.3, 114.4, 109.1, 55.5, 46.9, 39.3, 35.0, 32.4, 25.8, 25.1, 24.2. HRMS (ESI) m/z calculated for $C_{33}H_{31}N_2O_3$ $[M+H]^+$ = 503.2329, found = 503.2332.

5-(4-methoxyphenyl)-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3ab). 81% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.01-7.96 (m, 2H), 7.87 (s, 1H), 7.64-7.60 (m, 1H), 7.55 (d, J = 8.4 Hz, 1H), 7.53-7.48 (m, 1H), 7.46-7.38 (m, 3H), 7.30-7.25 (m, 3H), 7.07-7.02 (d, J = 9.0 Hz, 2H), 4.99 (dd, J = 7.6, 3.6 Hz, 1H), 3.90 (s, 3H), 3.55-3.23 (m, 2H), 2.48-2.29 (m, 2H), 2.25-2.17 (m, 2H), 1.94-1.86 (m, 1H), 1.83-1.71 (m, 1H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.3, 195.6, 159.1, 157.0, 150.9, 145.7, 137.1, 136.3, 132.9, 132.1, 128.9, 128.5, 128.3, 128.1, 126.9, 126.4, 124.4, 122.4, 114.4, 110.8, 55.4, 46.8, 36.5, 31.8, 29.0, 21.4. HRMS (ESI) m/z calculated for $C_{31}H_{27}N_2O_3$ $[M+H]^+$ = 475.2016, found = 475.2032.

5-(4-methoxyphenyl)-12-(2-oxo-2-phenylethyl)-3-phenyl-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3ac). 87% yield, red oily, d.r. = 1:1, **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.04-7.97 (m, 2H), 7.93-7.87 (m, 1H), 7.66-7.61 (m, 1H), 7.60-7.51 (m, 2H), 7.48-7.41 (m, 3H), 7.35-7.25 (m, 5H), 7.24-7.18 (m, 1H), 7.16-7.11 (m, 2H), 7.05-6.98 (m, 2H), 5.05 (dd, J = 7.4, 3.8 Hz, 1H), 5.07-4.97 (m, 1H), 3.90-3.84 (m, 3H), 3.67-3.49 (m, 1H), 3.42-3.00 (m, 2H), 2.76-2.57 (m, 2H), 2.53-2.40 (m, 2H). **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$): δ 198.3, 198.2, 194.8, 194.5, 159.1, 156.2, 156.1, 151.1, 150.7, 145.7, 145.7, 142.9, 142.8, 137.2, 137.0, 136.3, 136.2, 133.0, 132.9, 131.95, 131.6, 129.0, 128.7, 128.6, 128.6 128.5, 128.31, 128.28, 128.2, 128.1, 126.92, 126.86, 126.76, 126.7, 126.42, 126.39, 124.6, 124.5, 122.4, 122.2, 114.6, 114.3, 111.2, 110.1, 55.4, 46.9, 46.3, 43.6, 43.4, 40.1, 39.2, 36.5, 35.9, 32.0, 31.8. HRMS (ESI) m/z calculated for $C_{37}H_{31}N_2O_3$ $[M+H]^+$ = 551.2329, found = 551.2347.

5-(4-methoxyphenyl)-3,3,9-trimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3ad). 93% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.05-7.98 (m, 2H), 7.73 (s, 1H), 7.55-7.49 (m, 1H), 7.48-7.40 (m, 3H), 7.37 (s, 1H), 7.27 (d, *J* = 7.5 Hz, 3H), 7.06 (d, *J* = 8.9 Hz, 2H), 4.95 (dd, *J* = 7.4, 4.1 Hz, 1H), 3.92 (s, 3H), 3.39 (qd, *J* = 15.3, 5.9 Hz, 2H), 2.41 (s, 3H), 2.33-2.22 (m, 2H), 2.16-2.05 (m, 2H), 0.99 (s, 3H), 0.98 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.2, 195.3, 159.0, 155.4, 150.5, 144.2, 137.0, 135.6, 134.1, 132.9, 132.1, 131.1, 128.5, 128.3, 127.8, 126.3, 125.9, 122.1, 114.4, 109.6, 55.4, 50.1, 46.7, 42.4, 32.5, 31.9, 29.2, 27.4, 21.3. HRMS (ESI) m/z calculated for $C_{34}H_{33}N_2O_3$ $[M+H]^+$ = 517.2491, found = 517.2492.

9-methoxy-5-(4-methoxyphenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3ae). 80% yield, red oily, **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.00 (d, *J* = 7.8 Hz, 2H), 7.75 (s, 1H), 7.50 (t, *J* = 7.2 Hz, 1H), 7.47-7.40 (m, 3H), 7.25 (s, 1H), 7.10 (d, *J* = 9.0 Hz, 1H), 7.05 (d, *J* = 7.8 Hz, 2H), 6.91 (s, 1H), 4.96 (d, *J* = 6.0 Hz, 1H), 3.91 (s, 3H), 3.83 (s, 3H), 3.48-

3.30 (m, 2H), 2.32-2.22 (m, 2H), 2.14-2.04 (m, 2H), 0.98 (s, 6H). **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$): δ 198.2, 195.3, 159.0, 156.4, 155.4, 149.5, 141.4, 137.0, 135.2, 132.9, 132.1, 131.2, 129.5, 128.5, 128.3, 127.0, 122.4, 121.3, 114.4, 109.3, 104.9, 55.4, 55.4, 50.1, 46.6, 42.4, 32.5, 31.7, 29.1, 27.3. HRMS (ESI) m/z calculated for $C_{34}H_{33}N_2O_5$ $[M+H]^+$ = 533.2440, found = 533.2448.

5-(4-methoxyphenyl)-3,3-dimethyl-9-(methylthio)-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3af). 82% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.03-7.96 (m, 2H), 7.74 (s, 1H), 7.51 (t, J = 7.3 Hz, 1H), 7.47-7.40 (m, 3H), 7.38-7.31 (m, 2H), 7.28-7.25 (m, 2H), 7.05 (d, J = 8.8 Hz, 2H), 4.95 (dd, J = 7.6, 3.6 Hz, 1H), 3.91 (s, 3H), 3.51-3.30 (m, 2H), 2.50 (s, 3H), 2.34-2.21 (m, 2H), 2.17-2.01 (m, 2H), 0.99 (s, 3H), 0.98 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.2, 195.3, 159.1, 155.2, 150.6, 143.9, 137.0, 135.1, 134.6, 132.9, 132.0, 128.8, 128.5, 128.4, 128.3, 126.8, 122.9, 122.5, 114.4, 109.6, 55.4, 50.1, 46.6, 42.4, 32.5, 31.7, 29.1, 27.3, 16.0. HRMS (ESI) m/z calculated for $C_{34}H_{33}N_2O_3S$ $[M+H]^+$ = 549.2212, found = 549.2219.

9-fluoro-5-(4-methoxyphenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3ag). 88% yield, red oil, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.99 (d, J = 7.6 Hz, 2H), 7.76 (s, 1H), 7.58-7.49 (m, 2H), 7.48-7.39 (m, 2H), 7.28-7.17 (m, 4H), 7.06 (d, J = 8.8 Hz, 2H), 4.94 (dd, J = 7.6, 3.6 Hz, 1H), 3.92 (s, 3H), 3.53-3.31 (m, 2H), 2.34-2.21 (m, 2H), 2.18-2.03 (m, 2H), 0.99 (s, 3H), 0.97 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.2, 195.3, 159.3 (d, $J_{C\text{-}F}$ = 243.0 Hz), 159.1, 158.10, 155.3, 150.7 (d, $J_{C\text{-}F}$ = 3.0 Hz), 142.7, 136.9, 135.5 (d, $J_{C\text{-}F}$ = 5.0 Hz), 133.0, 133.0, 131.2, 130.3 (d, $J_{C\text{-}F}$ = 9.0 Hz), 128.6, 128.3, 126.6 (d, $J_{C\text{-}F}$ = 10.0 Hz), 123.4, 118.8 (d, $J_{C\text{-}F}$ = 26.0 Hz), 114.5, 110.1 (d, $J_{C\text{-}F}$ = 21.0 Hz), 109.6, 55.5, 50.1, 46.5, 42.4, 32.5, 31.8, 29.1, 27.4. **^{19}F NMR** (377 MHz, $CDCl_3$): δ -116.58 (dd, J = 13.9, 8.5 Hz). HRMS (ESI) m/z calculated for $C_{33}H_{30}FN_2O_3$ $[M+H]^+$ = 521.2240, found = 521.2256.

9-chloro-5-(4-methoxyphenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3ah). 86% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.04-7.94 (m, 2H), 7.72 (s, 1H), 7.57 (d, J = 2.4 Hz, 1H), 7.55-7.40 (m, 4H), 7.39-7.34 (m, 1H), 7.30-7.24 (m, 2H), 7.06 (d, J = 8.8 Hz, 2H), 4.93 (dd, J = 7.6, 3.6 Hz, 1H), 3.92 (s, 3H), 3.53-3.30 (m, 2H), 2.34-2.20 (m, 2H), 2.17-2.03 (m, 2H), 0.99 (s, 3H), 0.97 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.1, 195.4, 159.2, 155.2, 151.4, 144.1, 136.9, 135.2, 133.0, 131.9, 129.9, 129.8, 129.69, 129.65, 128.6, 128.3, 126.8, 125.5, 123.5, 114.5, 109.8, 55.5, 50.1, 46.5, 42.4, 32.5, 31.8, 29.2, 27.3. HRMS (ESI) m/z calculated for $C_{33}H_{30}BrN_2O_3$ $[M+H]^+$ = 581.1440, found = 581.1446.

9-bromo-5-(4-methoxyphenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3ai). 85% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.03-7.94 (m, 2H), 7.74 (d, J = 2.0 Hz, 1H), 7.72 (s, 1H), 7.55-7.47 (m, 2H), 7.46-7.38 (m, 3H), 7.29-7.24 (m, 2H), 7.06 (d, J = 9.2 Hz, 2H), 4.93 (dd, J = 7.6, 3.6 Hz, 1H), 3.92 (s, 3H), 3.53-3.30 (m, 2H), 2.34-2.21 (m, 2H), 2.17-2.00 (m, 2H), 0.99 (s, 3H), 0.97 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.1, 195.4, 159.1, 155.2, 151.4, 144.3, 136.9, 135.1, 133.0, 132.2, 131.9, 129.8, 128.8, 128.6, 128.3, 127.4, 123.5, 117.9, 114.5, 109.8, 55.5, 50.1, 46.5, 42.3, 32.5, 31.8, 29.2, 27.3. HRMS (ESI) m/z calculated for $C_{33}H_{30}ClN_2O_3$ $[M+H]^+$ = 537.1945, found = 537.1947.

8-fluoro-5-(4-methoxyphenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3aj). 87% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 7.6 Hz, 2H), 7.81 (s, 1H), 7.61-7.54 (m, 1H), 7.53-7.47 (m, 1H), 7.46-7.37 (m, 2H), 7.28-7.22 (m, 2H), 7.21-7.15 (m, 1H), 7.10-6.99 (m, 3H), 4.93 (dd, *J* = 7.2, 3.2 Hz, 1H), 3.92 (s, 3H), 3.40 (ddd, *J* = 19.0, 15.6, 5.6 Hz, 2H), 2.33 – 2.22 (m, 2H), 2.17 – 2.04 (m, 2H), 0.99 (s, 3H), 0.98 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.2, 195.4, 163.0 (d, J_{C-F} = 243.0 Hz), 159.1, 155.1, 151.9, 146.7 (d, J_{C-F} = 12.0 Hz), 136.9, 136.1, 132.9, 131.9, 131.0, 128.7 (d, J_{C-F} = 10.0 Hz), 128.5, 128.2, 123.2, 121.5 (d, J_{C-F} = 2.0 Hz), 114.49 (d, J_{C-F} = 25.0 Hz), 114.46, 111.9 (d, J_{C-F} = 21.0 Hz), 110.0, 55.4, 50.1, 46.5, 42.3, 32.5, 31.6, 29.1, 27.3. **^{19}F NMR** (377 MHz, $CDCl_3$): δ -110.81 – -111.02 (m). HRMS (ESI) m/z calculated for $C_{33}H_{30}FN_2O_3$ $[M+H]^+$ = 521.2240, found = 521.2252.

8-chloro-5-(4-methoxyphenyl)-3,3-dimethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3ak). 88% yield, red oily, **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.01-7.95 (m, 2H), 7.79 (s, 1H), 7.55 (d, *J* = 1.8 Hz, 1H), 7.54-7.49 (m, 2H), 7.45-7.40 (m, 2H), 7.26-7.19 (m, 3H), 7.10-7.04 (m, 2H), 4.93 (dd, *J* = 7.8, 3.6 Hz, 1H), 3.92 (s, 3H), 3.52-3.32 (m, 2H), 2.32-2.22 (m, 2H), 2.17-2.03 (m, 2H), 0.99 (s, 3H), 0.97 (s, 3H). **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$): δ 198.1, 195.4, 159.2, 155.1, 151.88, 146.2, 136.9, 136.0, 134.7, 133.0, 131.9, 131.0, 128.5, 128.3, 128.0, 127.1, 125.3, 124.6, 122.7, 114.5, 109.9, 55.5, 50.1, 46.5, 42.4, 32.5, 31.7, 29.2, 27.3. HRMS (ESI) m/z calculated for $C_{33}H_{30}ClN_2O_3$ $[M+H]^+$ = 537.1945, found = 537.1965.

5-(4-methoxyphenyl)-3,3,7,8-tetramethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3al). 80% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.03-7.97 (m, 2H), 7.74 (s, 1H), 7.54-7.48 (m, 1H), 7.46-7.40 (m, 2H), 7.35 (d, *J* = 8.4 Hz, 1H), 7.29 (d, *J* = 8.8 Hz, 2H), 7.13-7.03 (m, 3H), 3.54-3.30 (dd, *J* = 7.6, 3.6 Hz, 1H), 3.92 (s, 3H), 3.54-3.30 (m, 2H), 2.33 (s, 3H), 2.31-2.23 (m, 2H), 2.18 (s, 3H), 2.16 (s, 2H), 1.000 (s, 3H), 0.997 (s, 3H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.3, 195.4, 159.0, 155.4, 149.9, 144.4, 137.1, 136.8, 136.3, 134.9, 133.1, 132.8, 132.4, 129.6, 128.5, 128.3, 127.4, 124.5, 123.7, 120.7, 115.4, 114.2, 109.5, 55.48, 50.2, 46.8, 42.4, 32.5, 31.6, 29.1, 27.4, 20.4, 12.5. HRMS (ESI) m/z calculated for $C_{35}H_{35}N_2O_5$ $[M+H]^+$ = 531.2648, found = 531.2656.

5-(4-methoxyphenyl)-3,3,7,9-tetramethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3am). 88% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.08-8.00 (m, 2H), 7.69 (s, 1H), 7.55-7.48 (m, 1H), 7.47-7.41 (m, 2H), 7.29 (d, *J* = 9.2 Hz, 2H), 7.21 (s, 1H), 7.15 (s, 1H), 7.05 (d, *J* = 9.0 Hz, 2H), 4.96 (dd, *J* = 7.2, 4.8 Hz, 1H), 3.91 (s, 3H), 3.46-.34 (m, 2H), 2.37 (s, 3H), 2.34-2.23 (m, 2H), 2.21 (s, 3H), 2.16 (s, 2H), 1.00 (s, 6H). **^{13}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.3, 195.3, 158.9, 155.3, 149.4, 143.0, 137.0, 135.7, 135.5, 133.9, 132.8, 132.3, 131.3, 128.5, 128.3, 126.2, 123.6, 121.7, 114.1, 109.4, 55.4, 50.2, 46.8, 42.4, 32.5, 31.8, 29.1, 27.4, 21.3, 16.9. HRMS (ESI) m/z calculated for $C_{35}H_{35}N_2O_3$

$[M+H]^+$ = 531.2648, found = 531.2656.

5-(4-methoxyphenyl)-3,3,7,10-tetramethyl-12-(2-oxo-2-phenylethyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3an)

90% yield, red oily, **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.09-8.05 (m, 2H), 7.86 (s, 1H), 7.55-7.51 (m, 1H), 7.48-7.44 (m, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 7.2 Hz, 1H), 7.05 (d, *J* = 9.0 Hz, 2H), 6.99 (d, *J* = 7.1 Hz, 1H), 5.00 (dd, *J* = 8.4, 3.6 Hz, 1H), 3.92 (s, 3H), 3.49-3.31 m, 2H), 2.47 (s, 3H), 2.34-2.26 (m, 2H), 2.19 (s, 3H), 2.18-2.15 (m, 2H), 1.01 (s, 3H), 1.01 (s, 3H). **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$): δ 198.5, 195.3, 159.0, 155.3, 149.4, 144.8, 137.0, 133.8, 133.1, 132.9, 132.2, 131.3, 128.7, 128.6, 128.4, 125.4, 124.8, 120.8, 114.2, 109.5, 55.5, 50.2, 47.1, 42.4, 32.6, 32.3, 29.1, 27.4, 18.4, 17.0. HRMS (ESI) m/z calculated for $C_{35}H_{35}N_2O_5$ $[M+H]^+$ = 531.2648, found = 531.2658.

6-(4-methoxyphenyl)-8,8-dimethyl-11-(2-oxo-2-phenylethyl)-7,8,9,11-tetrahydro-[1,3]dioxolo[4',5':4,5]benzo[1,2-*b*]benzo[*g*][1,8]naphthyridin-10(6*H*)-one (3ao)

84% yield, red oily, **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.01 (d, *J* = 7.2 Hz, 2H), 7.61 (s, 1H), 7.54-7.48 (m, 1H), 7.46-7.37 (m, 2H), 7.23 (d, *J* = 8.4 Hz, 2H), 7.04 (d, *J* = 8.4 Hz, 2H), 6.86 (s, 2H), 5.95 (d, *J* = 3.2 Hz, 2H), 4.90 (t, *J* = 5.2 Hz, 1H), 3.90 (s, 3H), 3.45-3.23 (m, 2H), 2.35-2.19 (m, 2H), 2.15-1.96 (m, 2H), 0.98 (s, 7H). **^{113}C{^{1}H} NMR** (100 MHz, $CDCl_3$): δ 198.4, 195.3, 159.0, 155.3, 150.2, 149.7, 146.3, 143.5, 137.0, 135.3, 132.8, 132.1, 128.5, 128.3, 122.6, 119.6, 114.3, 109.4, 105.1, 102.3, 101.3, 55.4, 50.1, 46.7, 42.3, 32.5, 31.7, 29.1, 27.3. HRMS (ESI) m/z calculated for $C_{34}H_{31}N_2O_5$ $[M+H]^+$ = 547.2233, found = 547.2239.

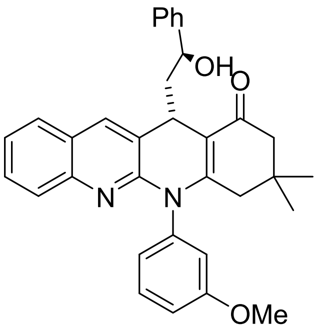
13-(4-methoxyphenyl)-11,11-dimethyl-8-(2-oxo-2-phenylethyl)-8,11,12,13-tetrahydrobenzo[*b*]naphtho[2,1-*g*][1,8]naphthyridin-9(10*H*)-one (3ap). 85% yield, red oily, **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.41 (d, *J* = 7.8 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 2H), 7.86 (s, 1H), 7.76 (d, *J* = 7.8 Hz, 1H), 7.58 (d, *J* = 8.8 Hz, 1H), 7.54-7.48 (m, 3H), 7.48-7.41 (m, 3H), 7.36 (d, *J* = 9.0 Hz, 2H), 7.14 (d, *J* = 9.0 Hz, 2H), 5.02 (dd, *J* = 7.8, 3.6 Hz, 1H), 3.98 (s, 3H), 3.53-3.33 (m, 2H), 2.36-2.25 (m, 2H), 2.17 (s, 2H), 1.02 (s, 6H). **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$): δ 198.3, 195.4, 159.1, 155.3, 150.2, 143.4, 137.1, 136.4, 133.6, 132.8, 132.2, 130.9, 128.5, 128.3, 127.5, 127.4, 126.4, 125.5, 124.7, 124.1, 123.7, 121.6, 114.4, 109.4, 55.55, 50.2, 46.8, 42.3, 32.5, 31.7, 29.2, 27.4. HRMS (ESI) m/z calculated for $C_{37}H_{33}N_2O_5$ $[M+H]^+$ = 553.2491, found = 553.2498.

5-(4-methoxyphenyl)-3,3-dimethyl-12-(2-oxopropyl)-3,4,5,12-tetrahydrodibenzo[*b*,*g*][1,8]naphthyridin-1(2*H*)-one (3aq). 51% yield, red oily, **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.97 (s, 1H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.59 (d, *J* = 8.4 Hz, 1H), 7.48-7.45 (m, 1H), 7.33-.29 (m, 1H), 7.27-7.26 (m, 2H), 7.09-7.03 (m, 2H), 4.78 (dd, *J* = 6.6, 4.2 Hz, 1H), 3.92 (s, 3H), 3.04-2.69 (m, 2H), 2.26 (s, 2H), 2.14-2.06 (m, 3H), 2.03 (s, 3H), 1.00 (s, 3H), 0.99 (s, 3H). **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$): δ 206.7, 195.3, 159.1, 155.2, 151.1, 145.6, 136.3, 132.0, 129.1, 128.1, 126.9, 126.4, 124.6, 122.8, 114.5, 109.7, 55.5, 51.6, 50.1, 42.4, 32.5, 30.7, 30.5, 29.4, 27.2. HRMS (ESI) m/z calculated for $C_{28}H_{29}N_2O_3$ $[M+H]^+$ = 441.2173, found = 441.2192.

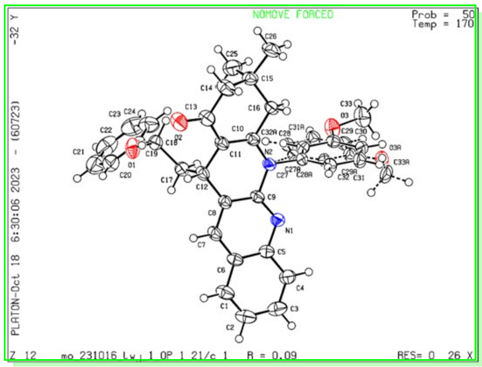
Ethyl 2-(6-(4-methoxyphenyl)-8,8-dimethyl-10-oxo-6,7,8,9,10,11-hexahydro-

dibenzo[*b*,*g*][1,8]naphthyridin-11-yl)acetate (3ar). 43% yield, red oily, **[1]H NMR** (600 MHz, $CDCl_3$): δ 8.00 (s, 1H), 7.69-7.66 (m, 1H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.51-7.46 (m, 1H), 7.34-7.30 (m, 1H), 7.25-7.21 (m, 2H), 7.08-7.03 (m, 2H), 4.80 (dd, *J* = 7.2, 5.6 Hz, 1H), 3.98 (q, *J* = 7.2 Hz, 2H), 3.93 (s, 3H), 2.78-2.62 (m, 2H), 2.28 (s, 2H), 2.16-2.06 (m, 2H), 1.06 (t, *J* = 7.2 Hz, 3H), 1.03 (s, 3H), 0.99 (s, 3H). **^{13}C{^{1}H} NMR** (150 MHz, $CDCl_3$): δ 195.1, 171.2, 159.2, 155.0, 151.0, 145.6, 136.5, 131.9, 131.0, 129.2, 128.1, 126.9, 126.4, 124.6, 122.1, 114.5, 109.7, 60.2, 55.5, 50.1, 42.5, 42.4, 32.4, 31.5, 29.5, 27.0, 14.1. HRMS (ESI) m/z calculated for $C_{29}H_{31}N_2O_4$ $[M+H]^+$ = 471.2278, found = 471.2296.

4. X-ray of 4



4



CCDC: **2306087**

Table 1 Crystal data and structure refinement for 4.

Identification code	mo_231016_LWJ_1_0m
Empirical formula	$C_{33}H_{32}N_2O_3$
Formula weight	504.60
Temperature/K	170.00
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	11.9232(3)
b/Å	10.4301(4)
c/Å	22.0572(8)
α/°	90
β/°	100.9190(10)
γ/°	90
Volume/$Å^3$	2693.38(16)
Z	4
ρ_{calc}g/cm^3	1.244
μ/mm^{-1}	0.080
F(000)	1072.0
Crystal size/mm^3	0.45 × 0.16 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.334 to 55.016
Index ranges	$-15 \le h \le 15$, $-13 \le k \le 13$, $-28 \le l \le 28$
Reflections collected	39856
Independent reflections	6193 [R_{int} = 0.0771, R_{sigma} = 0.0488]
Data/restraints/parameters	6193/284/421
Goodness-of-fit on F^2	1.173
Final R indexes [I>=2σ (I)]	R_1 = 0.0875, wR_2 = 0.1551
Final R indexes [all data]	R_1 = 0.1233, wR_2 = 0.1717
Largest diff. peak/hole / e Å^{-3}	0.24/-0.27

Table 2 Fractional Atomic Coordinates (×10^{4}) and Equivalent Isotropic Displacement Parameters (Å^{2}×10^{3}) for 4. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	-258.4(17)	6600(3)	2797.4(11)	52.8(6)
N1	4973.1(19)	4082(2)	3579.8(11)	34.9(5)
C1	3391(3)	1328(3)	2764.1(15)	46.4(8)
O2	552.8(17)	6844(3)	4092.3(11)	57.6(7)
N2	4383.1(18)	6009(2)	3945.9(11)	35.3(6)
C2	4283(3)	566(3)	2691.3(17)	52.4(9)
O3	7453(2)	8544(3)	3544.7(12)	44.8(7)
O3A	8354(9)	6412(11)	4761(5)	41(2)
C3	5411(3)	970(3)	2909.6(16)	51.3(9)
C4	5633(3)	2126(3)	3197.0(15)	42.1(7)
C5	4722(2)	2926(3)	3284.7(13)	33.8(6)
C6	3591(2)	2524(3)	3065.7(13)	34.6(6)
C7	2708(2)	3360(3)	3148.0(13)	35.7(6)
C8	2942(2)	4520(3)	3424.9(13)	31.2(6)
C9	4113(2)	4820(3)	3638.0(13)	31.1(6)
C10	3554(2)	6719(3)	4154.9(13)	32.7(6)
C11	2424(2)	6456(3)	3959.8(13)	33.5(6)
C12	2033(2)	5515(3)	3447.6(13)	34.3(6)
C13	1583(3)	7094(3)	4246.8(15)	44.4(8)
C14	1982(3)	8053(4)	4752.0(17)	54.4(10)
C15	3064(3)	8753(3)	4678.4(14)	39.3(7)
C16	3966(2)	7746(3)	4626.6(14)	38.3(7)
C17	1758(2)	6161(3)	2808.2(14)	38.7(7)
C18	791(2)	7150(3)	2704.6(15)	40.8(7)
C19	635(2)	7629(3)	2051.3(15)	41.2(7)
C20	-83(3)	7017(4)	1571.3(16)	51.3(8)
C21	-174(3)	7423(4)	969.0(18)	64.7(11)
C22	452(4)	8447(4)	833(2)	70.7(12)
C23	1183(4)	9062(4)	1303(2)	75.4(13)
C24	1273(3)	8656(3)	1909.9(19)	59.9(10)
C25	2860(3)	9616(3)	4109.7(17)	57.2(9)
C26	3483(3)	9584(3)	5250.5(16)	54.5(9)
C27	5598(3)	6337(3)	4126.9(17)	29.2(8)
C27A	5470(11)	6680(16)	3875(7)	28(2)
C28	5994(3)	7225(3)	3763.0(16)	29.5(7)
C28A	6333(11)	6286(15)	4338(7)	30(2)

Table 2 Fractional Atomic Coordinates (×10[4]) and Equivalent Isotropic Displacement Parameters (Å[2]×10[3]) for 4. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C29	7136(3)	7609(4)	3913.8(17)	30.7(8)
C29A	7422(12)	6764(17)	4335(8)	32(2)
C30	7850(3)	7077(3)	4413.2(17)	32.2(8)
C30A	7604(13)	7634(18)	3901(8)	33(2)
C31	7426(3)	6183(4)	4773.2(17)	38.6(8)
C31A	6743(11)	8043(15)	3435(7)	36(2)
C32	6291(3)	5805(3)	4638.4(17)	35.0(8)
C32A	5646(12)	7541(14)	3429(7)	31(2)
C33	8560(3)	9101(4)	3732(2)	54.4(11)
C33A	8150(14)	5417(16)	5168(8)	47(4)

Table 3 Anisotropic Displacement Parameters (Å[2]×10[3]) for 4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	26.4(11)	75.7(17)	56.8(14)	-0.6(13)	8.9(10)	-4.7(11)
N1	31.6(12)	30.4(13)	43.1(14)	-5.7(11)	7.6(10)	-2.6(10)
C1	50.2(19)	38.4(18)	55(2)	-13.5(15)	19.6(16)	-13.6(15)
O2	30.6(12)	79.8(18)	67.6(16)	-30.0(14)	22.5(11)	-12.0(11)
N2	23.7(11)	32.2(13)	49.9(14)	-13.5(11)	6.8(10)	-5.0(9)
C2	66(2)	34.7(18)	63(2)	-13.8(16)	30.0(18)	-10.7(16)
O3	38.9(14)	50.6(16)	44.4(15)	10.2(13)	7.0(11)	-13.6(12)
O3A	31(4)	42(5)	47(5)	9(4)	0(4)	-6(4)
C3	58(2)	37.9(18)	63(2)	-5.5(16)	25.2(18)	5.2(16)
C4	42.4(17)	35.2(17)	50.1(19)	-2.5(14)	12.3(14)	0.8(13)
C5	39.9(15)	28.0(14)	35.1(15)	-1.0(12)	11.1(12)	-1.9(12)
C6	41.7(16)	27.5(14)	37.0(16)	-4.0(12)	13.9(13)	-8.7(12)
C7	30.1(14)	36.3(16)	41.5(16)	-6.5(13)	8.8(12)	-11.6(12)
C8	26.6(13)	32.7(15)	35.1(15)	-3.5(12)	7.8(11)	-6.2(11)
C9	31.5(14)	28.0(14)	34.4(15)	-5.7(12)	7.8(11)	-6.7(11)
C10	30.9(14)	31.0(15)	37.4(15)	-5.9(12)	9.6(12)	-4.6(11)
C11	27.9(14)	37.5(16)	37.0(15)	-9.9(13)	11.2(11)	-7.9(12)
C12	26.0(13)	41.1(17)	37.0(15)	-10.6(13)	8.7(11)	-8.0(12)
C13	34.8(16)	53(2)	50.1(19)	-15.4(16)	19.3(14)	-9.1(14)
C14	44.1(18)	67(2)	58(2)	-29.4(19)	25.9(16)	-13.5(17)
C15	38.0(16)	37.2(17)	45.3(17)	-10.5(14)	15.0(13)	-2.5(13)

Table 3 Anisotropic Displacement Parameters (Å^2×10^3) for 4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C16	32.4(15)	36.2(16)	45.6(17)	-12.6(14)	5.7(13)	-4.7(12)
C17	31.0(15)	42.0(17)	43.8(17)	-11.1(14)	8.5(12)	1.6(13)
C18	27.5(14)	45.2(18)	50.3(18)	-9.4(15)	8.4(13)	-0.4(13)
C19	32.8(15)	35.4(16)	55.8(19)	-6.6(15)	9.5(14)	9.3(13)
C20	47.5(19)	53(2)	53(2)	-2.7(17)	8.3(16)	3.9(16)
C21	66(2)	71(3)	56(2)	-1(2)	8.1(19)	14(2)
C22	79(3)	74(3)	64(3)	11(2)	25(2)	29(2)
C23	94(3)	47(2)	95(3)	17(2)	41(3)	8(2)
C24	69(2)	41(2)	72(3)	-3.9(19)	19(2)	-2.3(18)
C25	66(2)	44(2)	61(2)	-3.1(18)	10.5(18)	7.4(18)
C26	53(2)	55(2)	58(2)	-29.3(18)	17.4(17)	-7.7(17)
C27	23.7(16)	27.2(18)	35.4(19)	-2.9(15)	2.0(14)	-2.8(13)
C27A	23(4)	26(4)	35(5)	-7(4)	4(4)	-1(4)
C28	30.2(16)	27.5(16)	29.7(17)	0.7(14)	3.1(13)	1.3(13)
C28A	26(4)	28(4)	33(4)	2(4)	1(4)	-1(3)
C29	33.2(18)	27.7(16)	32.5(16)	-1.4(13)	9.2(15)	-3.3(16)
C29A	28(4)	31(4)	37(4)	2(3)	3(3)	-5(3)
C30	26.9(17)	29.9(18)	39.1(18)	-0.7(15)	4.2(15)	-1.5(14)
C30A	31(4)	31(4)	38(4)	0(4)	8(4)	-5(4)
C31	34.5(18)	36.9(19)	40.4(18)	6.5(15)	-2.5(15)	-1.2(15)
C31A	35(4)	34(4)	38(4)	1(4)	4(4)	-7(4)
C32	32.7(17)	32.2(18)	38.5(19)	8.6(16)	3.0(14)	-5.0(14)
C32A	28(4)	29(4)	36(4)	-1(4)	3(4)	0(4)
C33	45(2)	58(3)	61(3)	14(2)	11.0(19)	-20(2)
C33A	35(8)	45(9)	53(9)	15(8)	-8(7)	9(7)

Table 4 Bond Lengths for 4.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C18	1.426(3)	C12	C17	1.541(4)
N1	C5	1.376(4)	C13	C14	1.506(4)
N1	C9	1.308(3)	C14	C15	1.517(4)
C1	C2	1.361(5)	C15	C16	1.524(4)
C1	C6	1.413(4)	C15	C25	1.526(5)
O2	C13	1.239(3)	C15	C26	1.535(4)
N2	C9	1.421(3)	C17	C18	1.532(4)
N2	C10	1.382(3)	C18	C19	1.503(5)

Table 4 Bond Lengths for 4.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N2	C27	1.469(4)	C19	C20	1.384(5)
N2	C27A	1.507(13)	C19	C24	1.383(5)
C2	C3	1.404(5)	C20	C21	1.378(5)
O3	C29	1.369(4)	C21	C22	1.369(6)
O3	C33	1.430(4)	C22	C23	1.379(6)
O3A	C29A	1.364(14)	C23	C24	1.389(6)
O3A	C33A	1.422(14)	C27	C28	1.366(5)
C3	C4	1.365(4)	C27	C32	1.382(5)
C4	C5	1.411(4)	C27A	C28A	1.369(14)
C5	C6	1.407(4)	C27A	C32A	1.377(15)
C6	C7	1.404(4)	C28	C29	1.397(5)
C7	C8	1.361(4)	C28A	C29A	1.391(15)
C8	C9	1.421(4)	C29	C30	1.375(5)
C8	C12	1.509(4)	C29A	C30A	1.365(15)
C10	C11	1.363(4)	C30	C31	1.381(5)
C10	C16	1.509(4)	C30A	C31A	1.376(15)
C11	C12	1.502(4)	C31	C32	1.387(5)
C11	C13	1.445(4)	C31A	C32A	1.407(15)

Table 5 Bond Angles for 4.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C9	N1	C5	117.3(2)	C14	C15	C25	111.5(3)
C2	C1	C6	120.3(3)	C14	C15	C26	109.6(3)
C9	N2	C27	117.1(2)	C16	C15	C25	110.5(3)
C9	N2	C27A	118.5(7)	C16	C15	C26	109.0(3)
C10	N2	C9	121.0(2)	C25	C15	C26	108.6(3)
C10	N2	C27	121.0(2)	C10	C16	C15	113.5(2)
C10	N2	C27A	118.0(7)	C18	C17	C12	117.0(2)
C1	C2	C3	120.2(3)	O1	C18	C17	111.3(3)
C29	O3	C33	117.5(3)	O1	C18	C19	108.6(2)
C29A	O3A	C33A	114.7(11)	C19	C18	C17	108.6(2)
C4	C3	C2	120.9(3)	C20	C19	C18	121.8(3)
C3	C4	C5	120.0(3)	C24	C19	C18	120.0(3)
N1	C5	C4	118.6(3)	C24	C19	C20	118.1(3)
N1	C5	C6	122.1(3)	C21	C20	C19	121.4(4)
C6	C5	C4	119.3(3)	C22	C21	C20	120.2(4)
C5	C6	C1	119.3(3)	C21	C22	C23	119.5(4)

Table 5 Bond Angles for 4.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C7	C6	C1	123.0(3)	C22	C23	C24	120.3(4)
C7	C6	C5	117.6(3)	C19	C24	C23	120.6(4)
C8	C7	C6	121.0(3)	C28	C27	N2	115.5(3)
C7	C8	C9	116.7(3)	C28	C27	C32	122.2(3)
C7	C8	C12	122.7(2)	C32	C27	N2	122.3(3)
C9	C8	C12	120.3(2)	C28A	C27A	N2	108.8(10)
N1	C9	N2	116.7(2)	C28A	C27A	C32A	122.3(12)
N1	C9	C8	125.3(2)	C32A	C27A	N2	128.9(11)
N2	C9	C8	118.0(2)	C27	C28	C29	118.9(3)
N2	C10	C16	116.8(2)	C27A	C28A	C29A	117.3(13)
C11	C10	N2	120.9(2)	O3	C29	C28	115.4(3)
C11	C10	C16	122.2(2)	O3	C29	C30	124.4(3)
C10	C11	C12	121.1(2)	C30	C29	C28	120.2(3)
C10	C11	C13	119.7(3)	O3A	C29A	C28A	122.6(12)
C13	C11	C12	119.2(2)	O3A	C29A	C30A	116.4(12)
C8	C12	C17	107.4(2)	C30A	C29A	C28A	121.0(12)
C11	C12	C8	110.6(2)	C29	C30	C31	119.6(3)
C11	C12	C17	112.6(2)	C29A	C30A	C31A	122.3(14)
O2	C13	C11	121.1(3)	C30	C31	C32	121.2(3)
O2	C13	C14	120.1(3)	C30A	C31A	C32A	116.9(13)
C11	C13	C14	118.8(3)	C27	C32	C31	117.9(3)
C13	C14	C15	113.4(2)	C27A	C32A	C31A	120.2(13)
C14	C15	C16	107.6(3)				

Table 6 Torsion Angles for 4.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C18	C19	C20	-33.0(4)	C11	C12	C17	C18	-62.1(3)
O1	C18	C19	C24	151.2(3)	C11	C13	C14	C15	30.9(5)
N1	C5	C6	C1	179.8(3)	C12	C8	C9	N1	-172.4(3)
N1	C5	C6	C7	1.1(4)	C12	C8	C9	N2	8.4(4)
C1	C2	C3	C4	0.0(5)	C12	C11	C13	O2	2.5(5)
C1	C6	C7	C8	-178.0(3)	C12	C11	C13	C14	-178.9(3)
O2	C13	C14	C15	-150.5(3)	C12	C17	C18	O1	-58.6(3)
N2	C10	C11	C12	-8.6(4)	C12	C17	C18	C19	-178.1(2)
N2	C10	C11	C13	171.6(3)	C13	C11	C12	C8	-152.1(3)
N2	C10	C16	C15	161.1(3)	C13	C11	C12	C17	87.7(3)
N2	C27	C28	C29	178.6(3)	C13	C14	C15	C16	-54.7(4)

Table 6 Torsion Angles for 4.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N2	C27	C32	C31	-179.6(3)	C13	C14	C15	C25	66.6(4)
N2	C27A	C28A	C29A	177.3(14)	C13	C14	C15	C26	-173.2(3)
N2	C27A	C32A	C31A	-178.5(14)	C14	C15	C16	C10	50.1(3)
C2	C1	C6	C5	0.6(5)	C16	C10	C11	C12	174.3(3)
C2	C1	C6	C7	179.2(3)	C16	C10	C11	C13	-5.5(5)
C2	C3	C4	C5	0.8(5)	C17	C18	C19	C20	88.2(3)
O3	C29	C30	C31	176.8(4)	C17	C18	C19	C24	-87.5(3)
O3A	C29A	C30A	C31A	178.3(18)	C18	C19	C20	C21	-176.5(3)
C3	C4	C5	N1	179.5(3)	C18	C19	C24	C23	176.4(3)
C3	C4	C5	C6	-0.9(5)	C19	C20	C21	C22	0.1(6)
C4	C5	C6	C1	0.2(4)	C20	C19	C24	C23	0.5(5)
C4	C5	C6	C7	-178.5(3)	C20	C21	C22	C23	0.7(6)
C5	N1	C9	N2	179.7(2)	C21	C22	C23	C24	-0.9(6)
C5	N1	C9	C8	0.5(4)	C22	C23	C24	C19	0.3(6)
C5	C6	C7	C8	0.6(4)	C24	C19	C20	C21	-0.7(5)
C6	C1	C2	C3	-0.7(5)	C25	C15	C16	C10	-71.8(3)
C6	C7	C8	C9	-1.6(4)	C26	C15	C16	C10	168.9(3)
C6	C7	C8	C12	171.7(3)	C27	N2	C9	N1	4.5(4)
C7	C8	C9	N1	1.1(4)	C27	N2	C9	C8	-176.2(3)
C7	C8	C9	N2	-178.1(3)	C27	N2	C10	C11	176.4(3)
C7	C8	C12	C11	159.2(3)	C27	N2	C10	C16	-6.3(4)
C7	C8	C12	C17	-77.5(3)	C27	C28	C29	O3	-177.0(3)
C8	C12	C17	C18	175.9(2)	C27	C28	C29	C30	1.4(5)
C9	N1	C5	C4	178.0(3)	C27A	N2	C9	N1	33.2(7)
C9	N1	C5	C6	-1.6(4)	C27A	N2	C9	C8	-147.4(7)
C9	N2	C10	C11	-14.4(4)	C27A	N2	C10	C11	147.3(7)
C9	N2	C10	C16	162.9(3)	C27A	N2	C10	C16	-35.4(7)
C9	N2	C27	C28	103.4(3)	C27A	C28A	C29A	O3A	-178.1(17)
C9	N2	C27	C32	-77.9(4)	C27A	C28A	C29A	C30A	3(3)
C9	N2	C27A	C28A	-90.8(13)	C28	C27	C32	C31	-1.0(6)
C9	N2	C27A	C32A	88.3(18)	C28	C29	C30	C31	-1.5(6)
C9	C8	C12	C11	-27.7(4)	C28A	C27A	C32A	C31A	0(3)
C9	C8	C12	C17	95.6(3)	C28A	C29A	C30A	C31A	-3(3)
C10	N2	C9	N1	-165.1(3)	C29	C30	C31	C32	0.3(6)
C10	N2	C9	C8	14.2(4)	C29A	C30A	C31A	C32A	1(3)
C10	N2	C27	C28	-87.0(4)	C30	C31	C32	C27	0.9(6)
C10	N2	C27	C32	91.7(4)	C30A	C31A	C32A	C27A	0(3)
C10	N2	C27A	C28A	107.0(12)	C32	C27	C28	C29	-0.1(5)

Table 6 Torsion Angles for 4.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C10	N2	C27A	C32A	-73.9(18)	C32A	C27A	C28A	C29A	-2(3)
C10	C11	C12	C8	28.1(4)	C33	O3	C29	C28	171.2(3)
C10	C11	C12	C17	-92.1(3)	C33	O3	C29	C30	-7.2(6)
C10	C11	C13	O2	-177.7(3)	C33A	O3A	C29A	C28A	7(3)
C10	C11	C13	C14	0.9(5)	C33A	O3A	C29A	C30A	-174.3(18)
C11	C10	C16	C15	-21.7(4)					

Table 7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 4.

Atom	*x*	*y*	*z*	U(eq)
H1	-214.01	6431.12	3173.54	79
H1A	2630.13	1053.58	2611.39	56
H2	4142.46	-241.56	2492.19	63
H3	6027.6	431.04	2856.56	62
H4	6400	2392.94	3337.78	51
H7	1936.41	3110.29	3008.31	43
H12	1329.39	5073.99	3526.48	41
H14A	2120.25	7603.54	5154.5	65
H14B	1368.45	8689.95	4757.43	65
H16A	4638.93	8175.48	4515.21	46
H16B	4214.38	7336.16	5034.89	46
H17A	2461.07	6587.68	2733.23	46
H17B	1564.87	5480.29	2493.05	46
H18	998.05	7884.31	2995.9	49
H20	-521.9	6304.33	1658.65	62
H21	-672.73	6989.03	647.11	78
H22	382.8	8733.13	418.8	85
H23	1628.23	9765.82	1210.82	90
H24	1775.99	9087.31	2230.63	72
H25A	3568.14	10067.98	4080.15	86
H25B	2262.45	10242.3	4144.75	86
H25C	2617.84	9093.03	3739.01	86
H26A	3615.36	9041.3	5619.88	82
H26B	2905.1	10232.04	5287.82	82
H26C	4197.96	10009.69	5209.32	82
H28	5500.85	7574.97	3413.17	35
H28A	6194.82	5710.13	4649.44	36

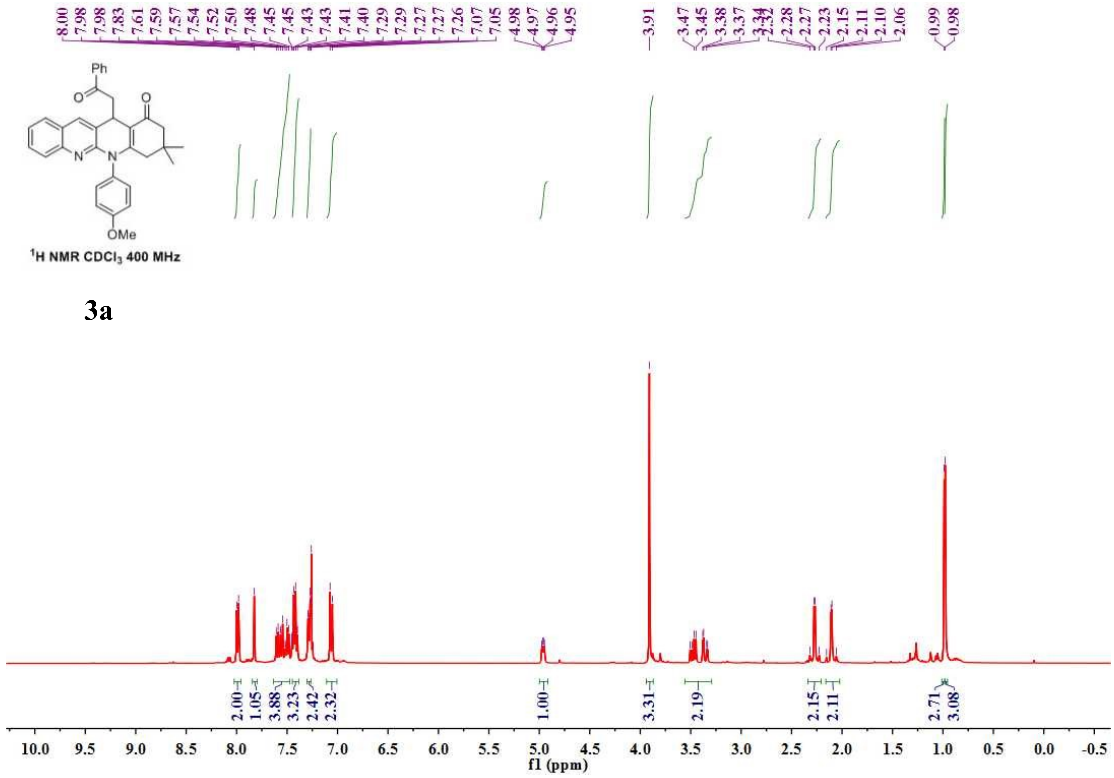
Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 4.

Atom	*x*	*y*	*z*	U(eq)
H30	8630.25	7323.69	4510.16	39
H30A	8351.95	7967.87	3921.77	39
H31	7920.42	5821.06	5119.12	46
H31A	6883.21	8638.32	3131.96	43
H32	5998.03	5199.53	4890.07	42
H32A	5025.31	7796.29	3115.83	38
H33A	8614.64	9880.26	3490.76	82
H33B	9143.34	8486.56	3660.39	82
H33C	8680.64	9316.98	4171.49	82
H33D	7701.13	4735.3	4929.83	70
H33E	7727.11	5762.54	5471.25	70
H33F	8880.95	5066.7	5381.85	70

Table 8 Atomic Occupancy for 4.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
O3	0.823(3)	O3A	0.177(3)	C27	0.823(3)
C27A	0.177(3)	C28	0.823(3)	H28	0.823(3)
C28A	0.177(3)	H28A	0.177(3)	C29	0.823(3)
C29A	0.177(3)	C30	0.823(3)	H30	0.823(3)
C30A	0.177(3)	H30A	0.177(3)	C31	0.823(3)
H31	0.823(3)	C31A	0.177(3)	H31A	0.177(3)
C32	0.823(3)	H32	0.823(3)	C32A	0.177(3)
H32A	0.177(3)	C33	0.823(3)	H33A	0.823(3)
H33B	0.823(3)	H33C	0.823(3)	C33A	0.177(3)
H33D	0.177(3)	H33E	0.177(3)	H33F	0.177(3)

5. NMR Spectra



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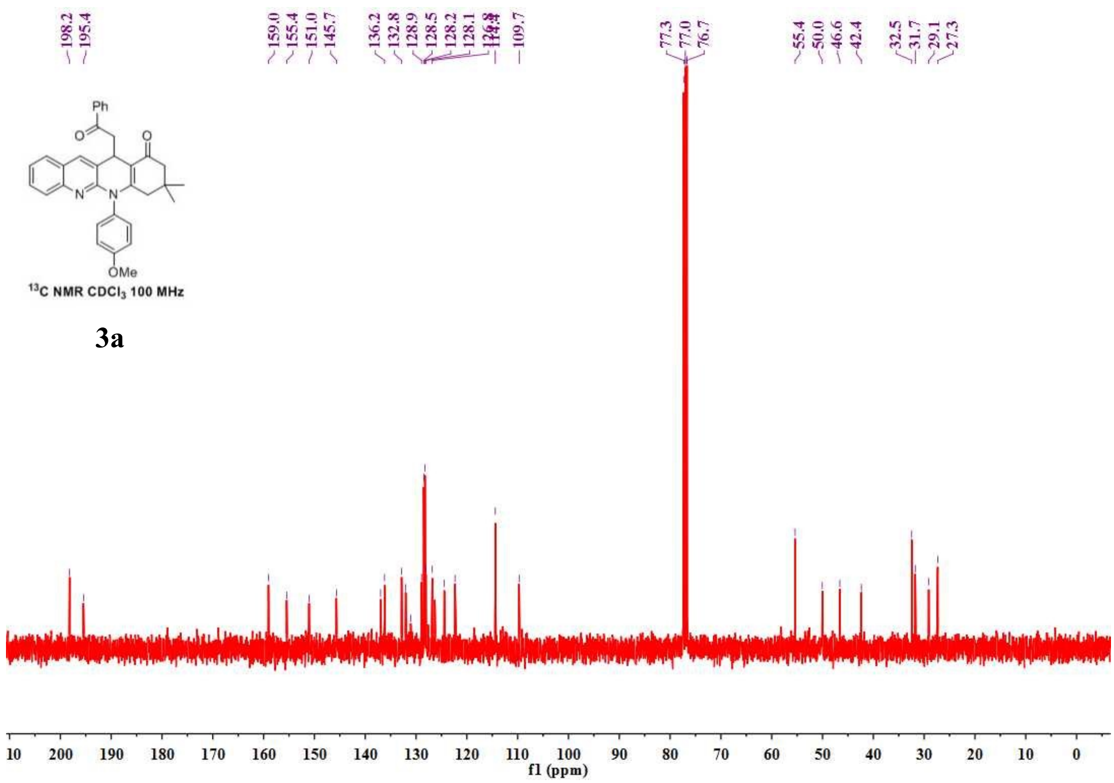

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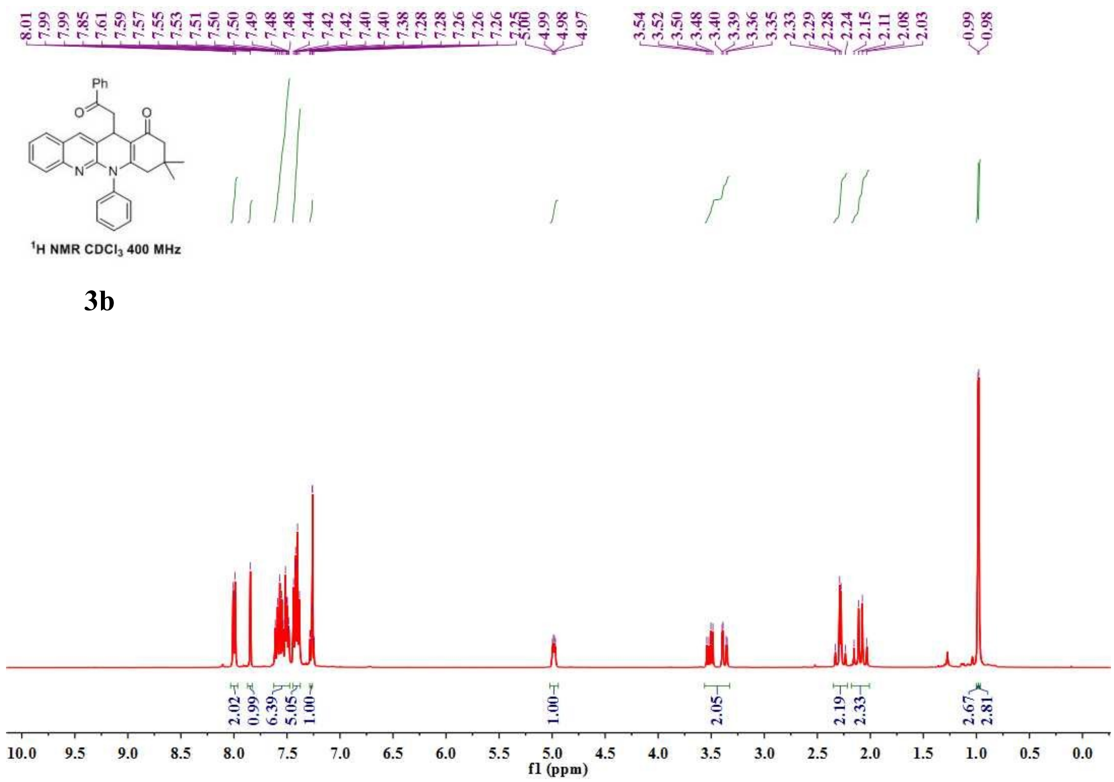

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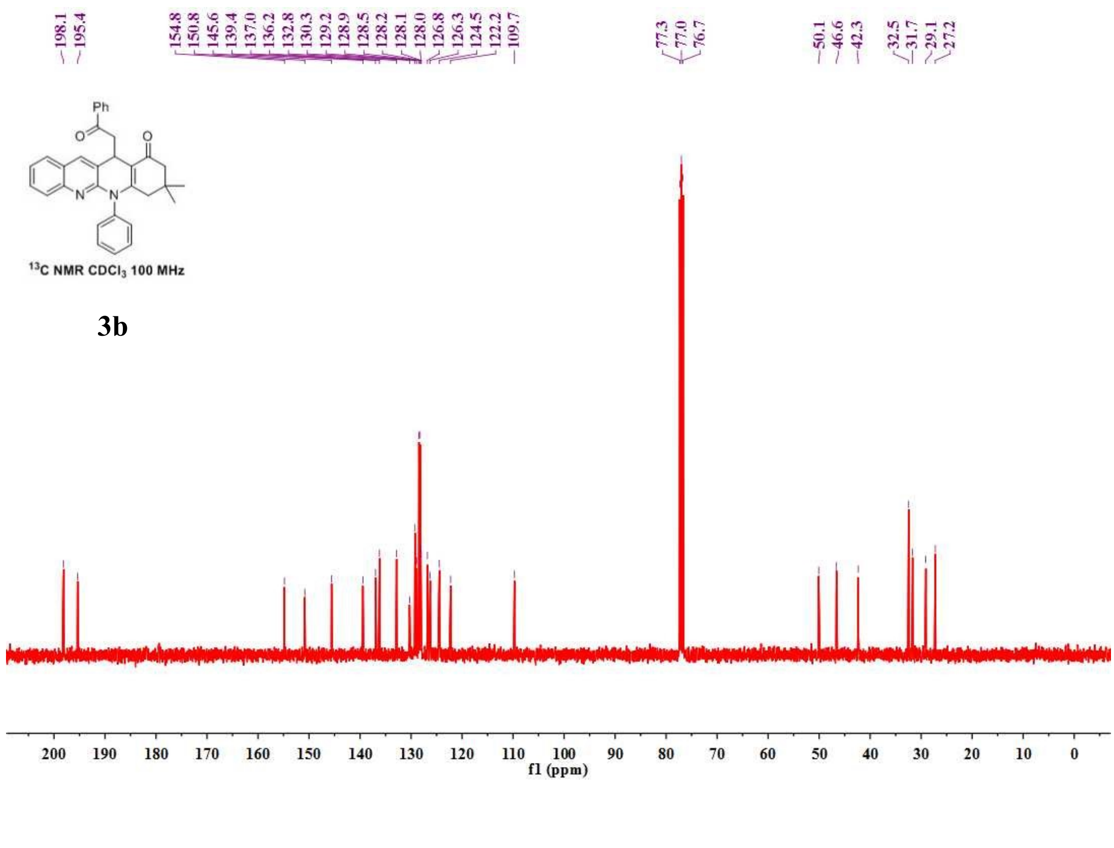

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128.2
128.1
128.0
126.8
126.3
124.5
122.2
109.7
77.3
77.0
76.7
50.1
46.6
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N
N
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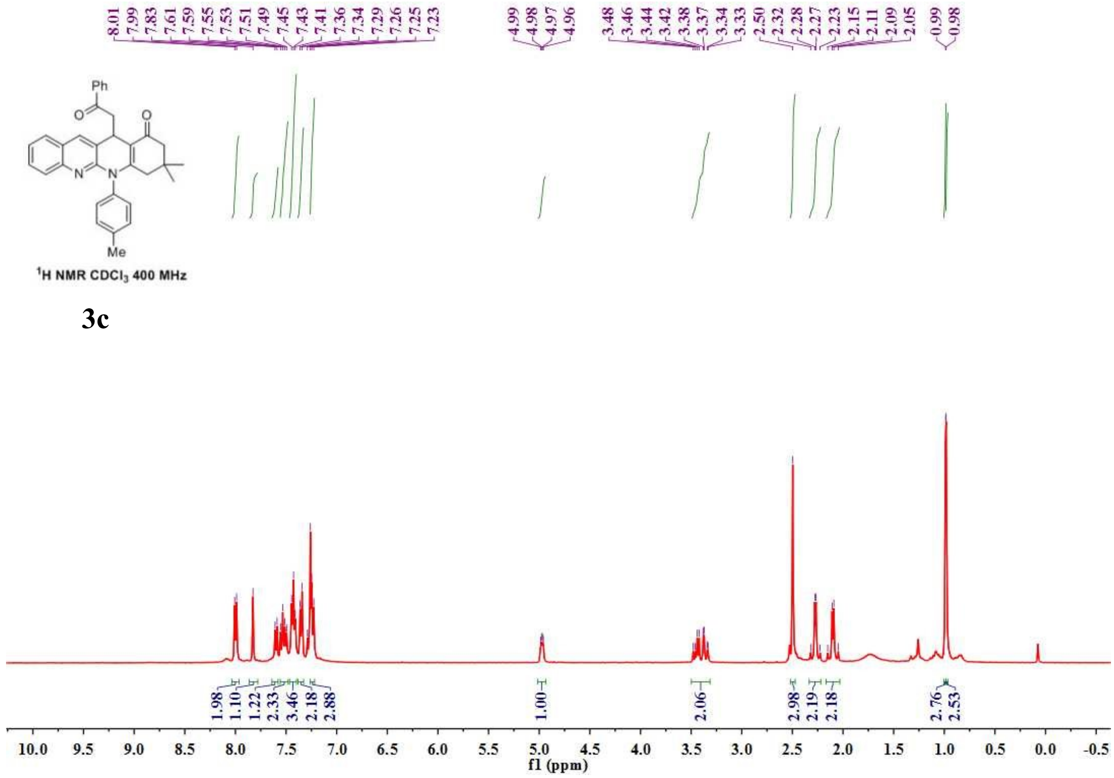
3b
f1 (ppm)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3.48 3.46 3.44 3.42 3.38 3.37 3.34 3.33 2.50 2.32 2.28 2.27 2.23 2.15 2.11 2.09 2.05
0.99 0.98
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O
N
Me
¹H NMR CDCl₃ 400 MHz
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1.00
2.06
2.98 2.19 2.18
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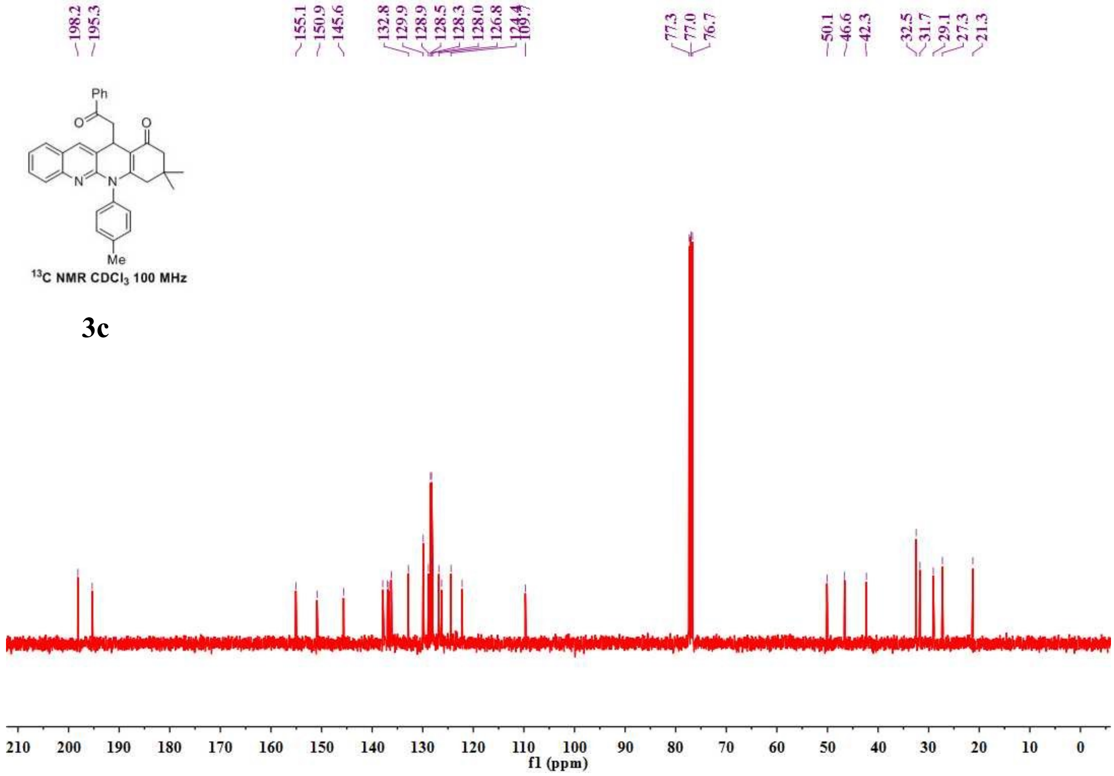
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32.5 31.7 29.1 27.3 21.3
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Me
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3c
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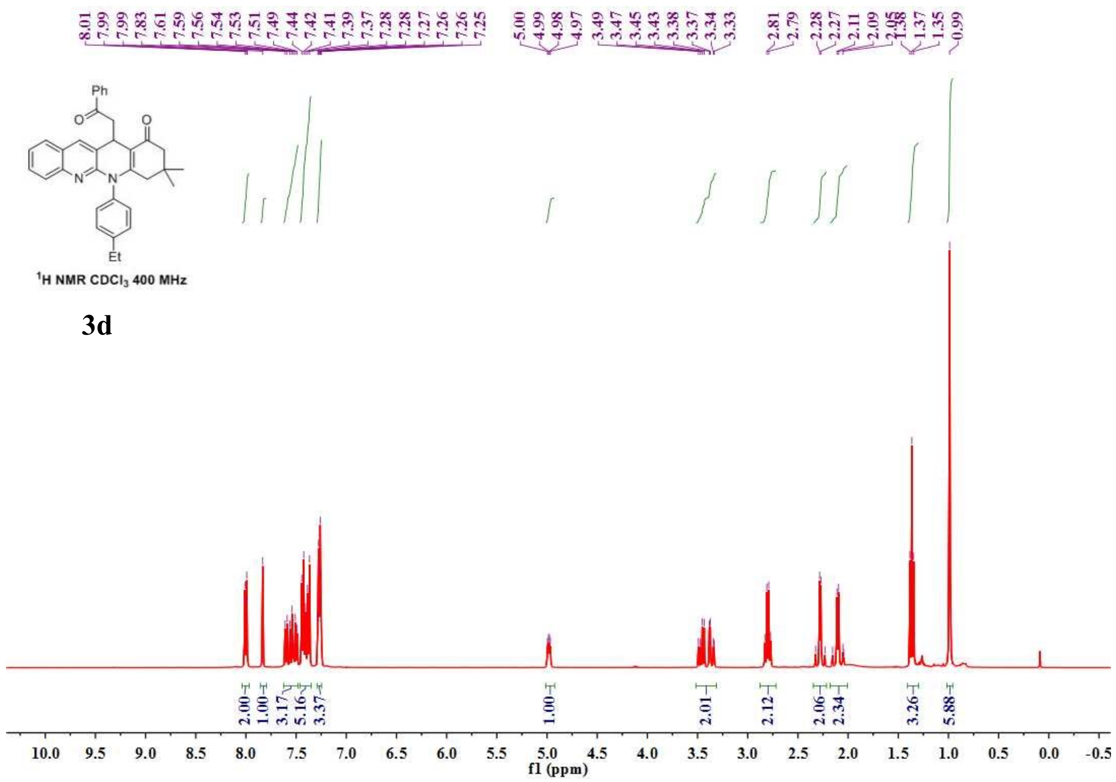
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5.00 4.99 4.98 4.97
3.49 3.47 3.45 3.43 3.38 3.37 3.34 3.33
2.81 2.79 2.28 2.27 2.11 2.09 2.05 1.38 1.37 1.35 0.99
Ph
O
N
Et
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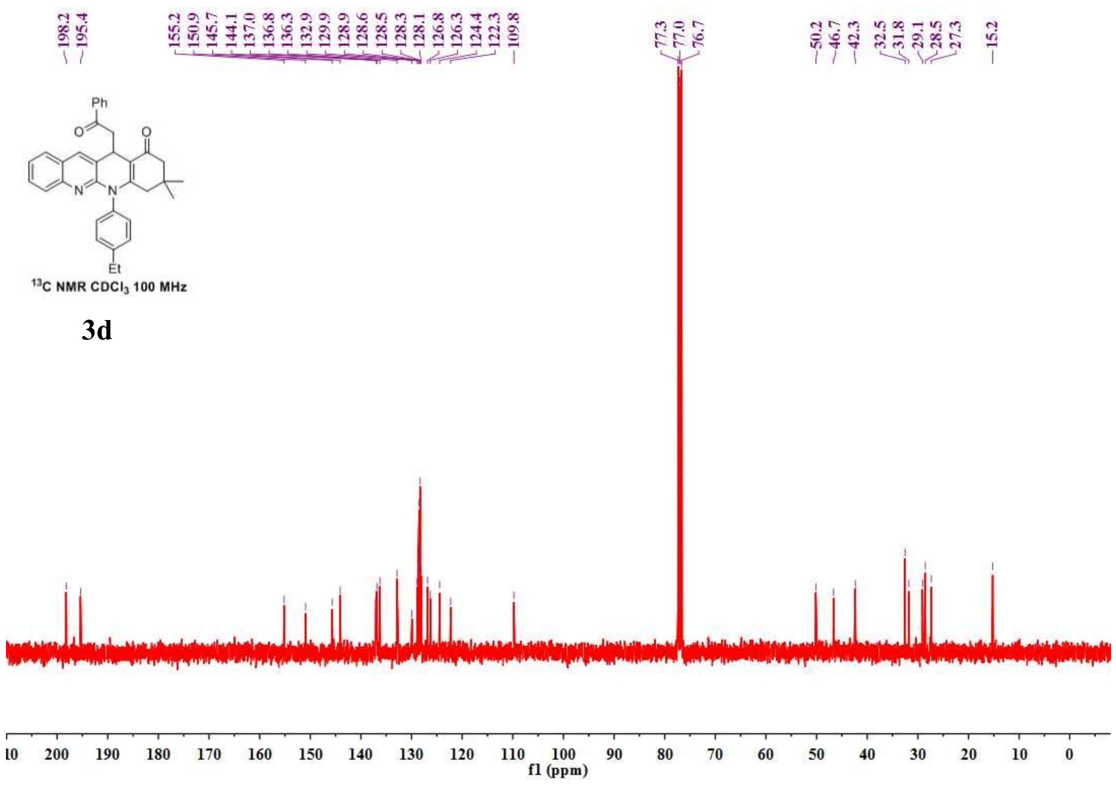
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77.3 77.0 76.7
50.2 46.7 42.3 32.5 31.8 29.1 28.5 27.3 15.2
Ph
O
N
Et
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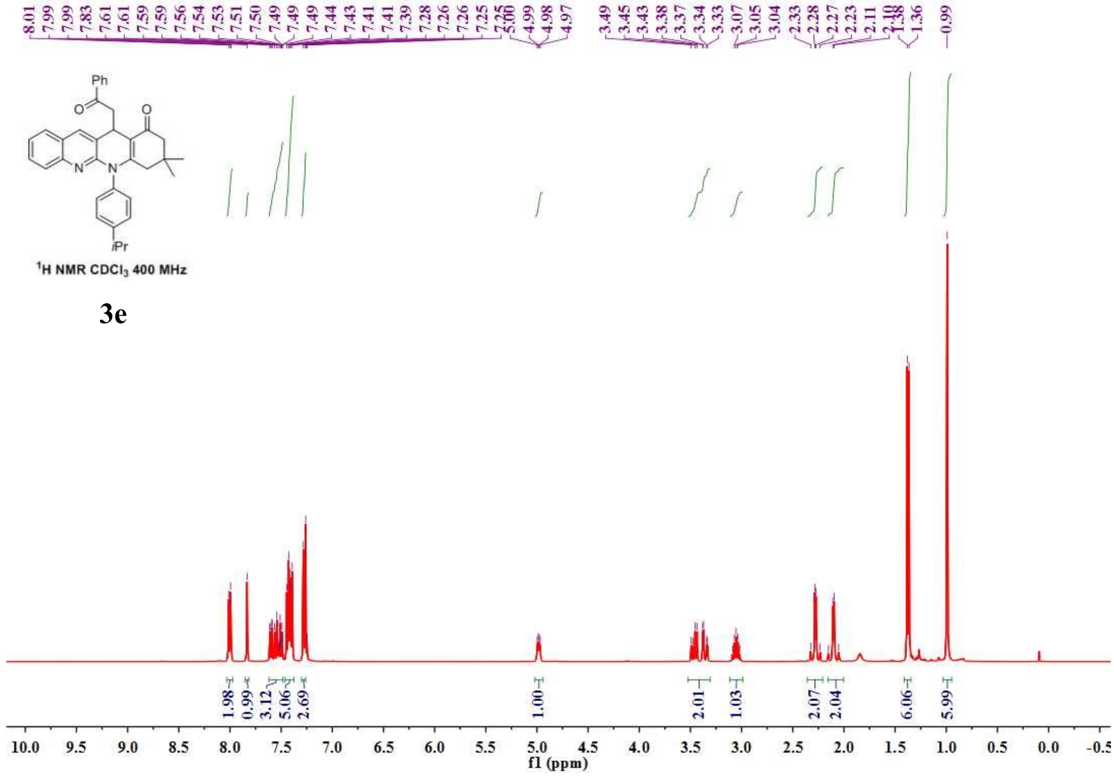
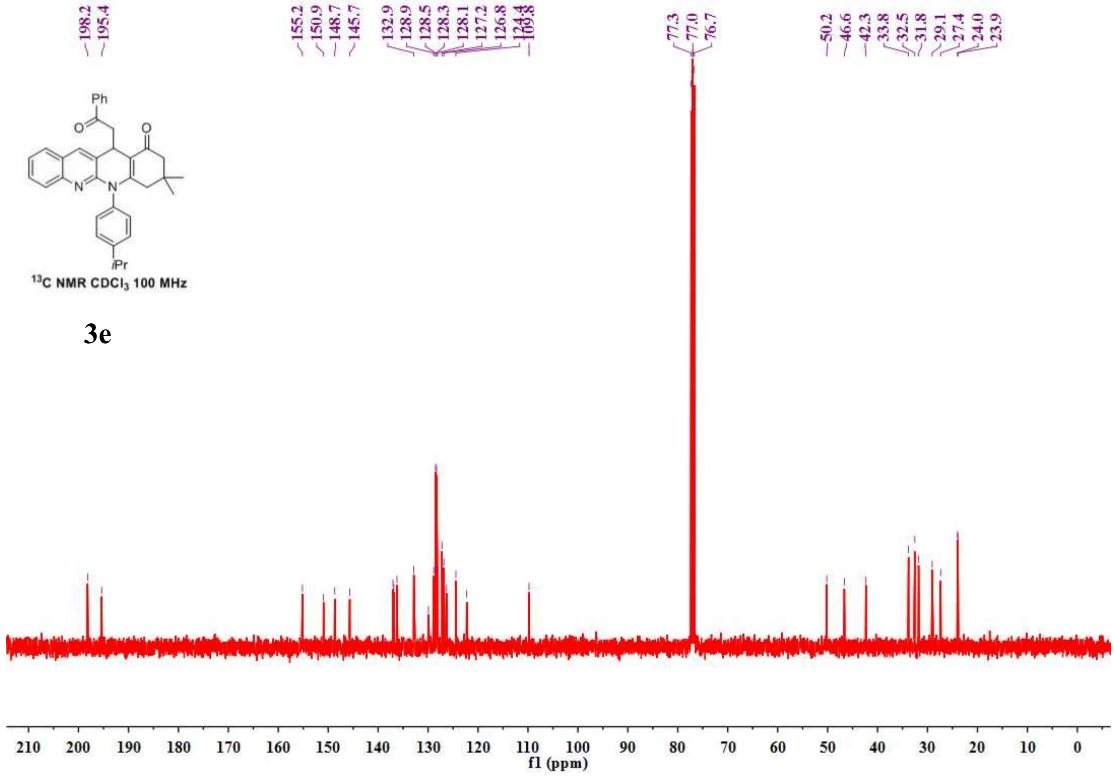
3d
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



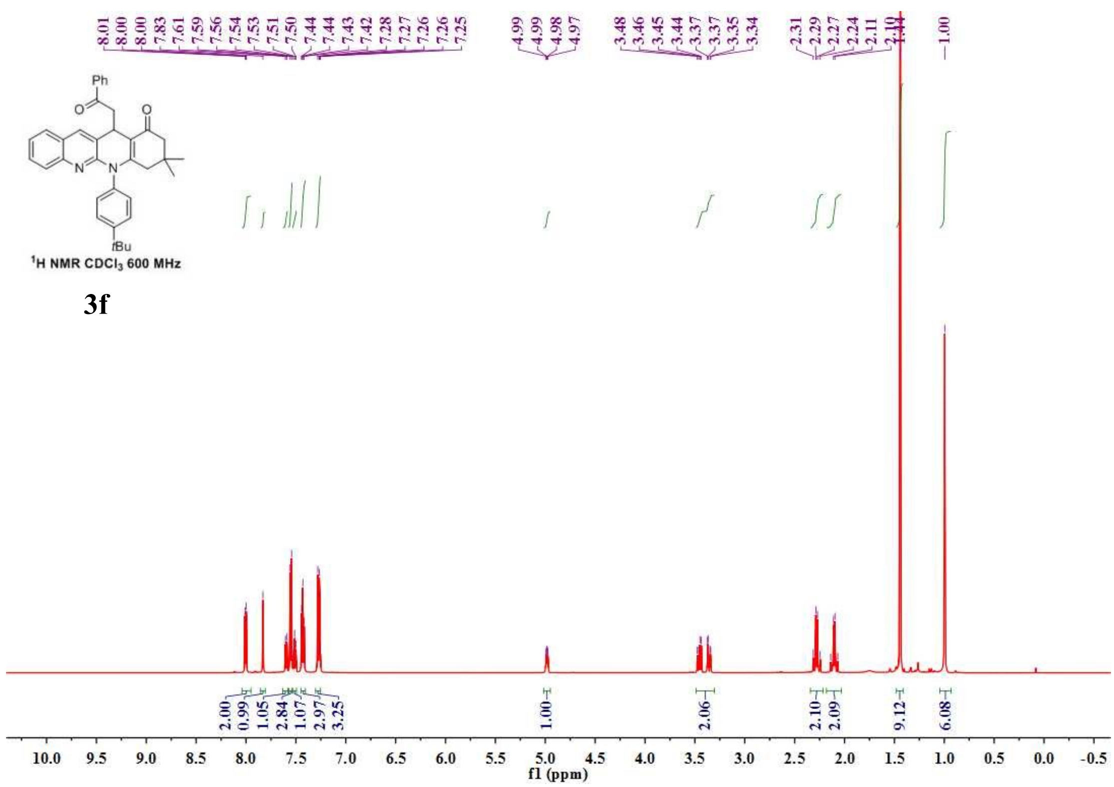
Ph
O
O
N
N
iPr
1H NMR CDCl3 400 MHz
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

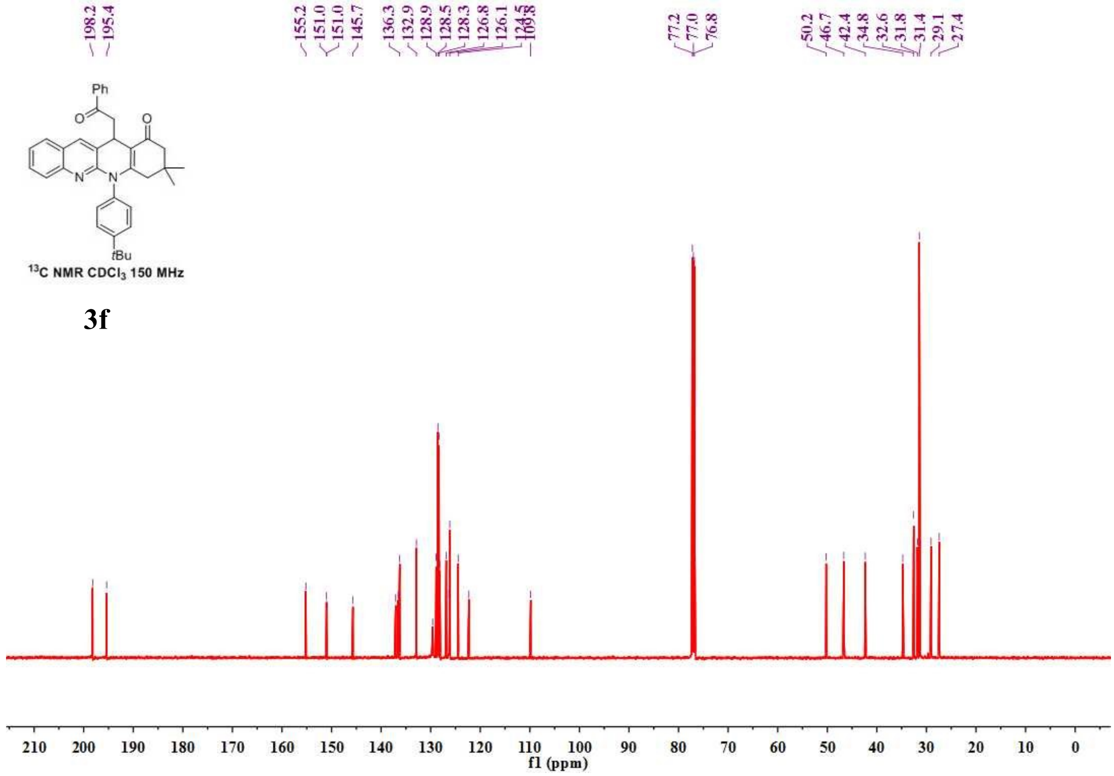
3e

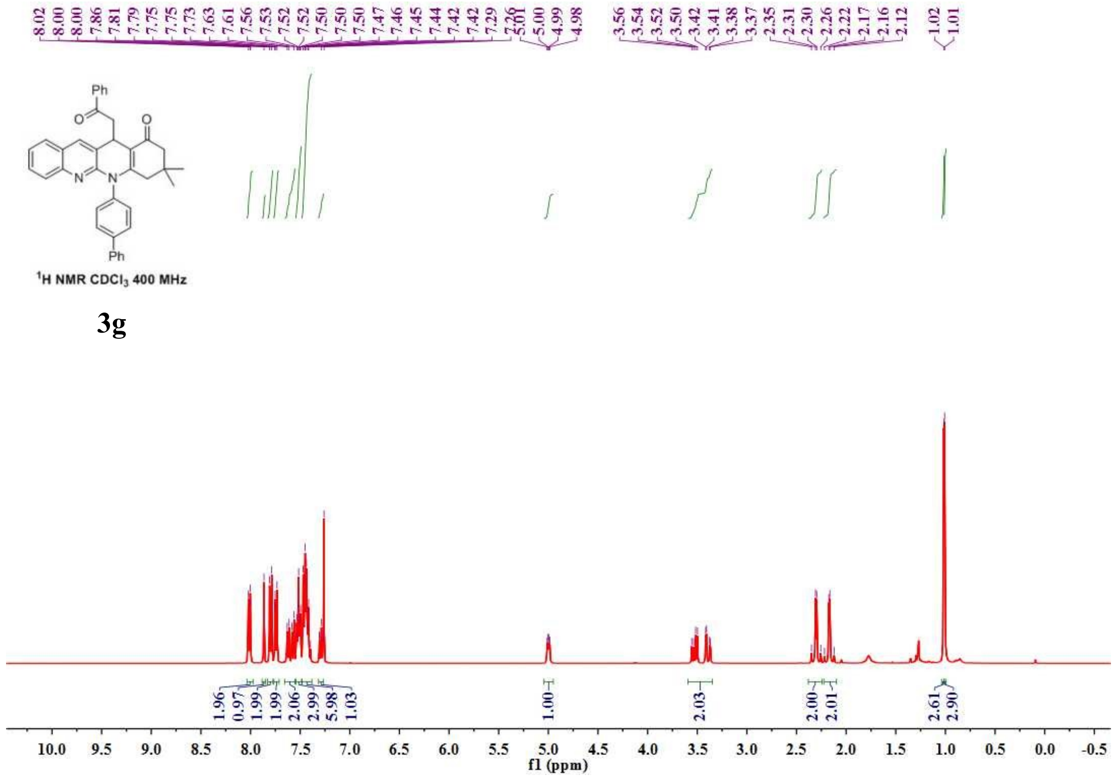


198.2
195.4
155.2
150.9
148.7
145.7
132.9
128.9
128.5
128.3
128.1
127.2
126.8
77.3
77.0
76.7
50.2
46.6
42.3
33.8
32.5
31.8
29.1
27.4
24.0
23.9
13C NMR CDCl3 100 MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

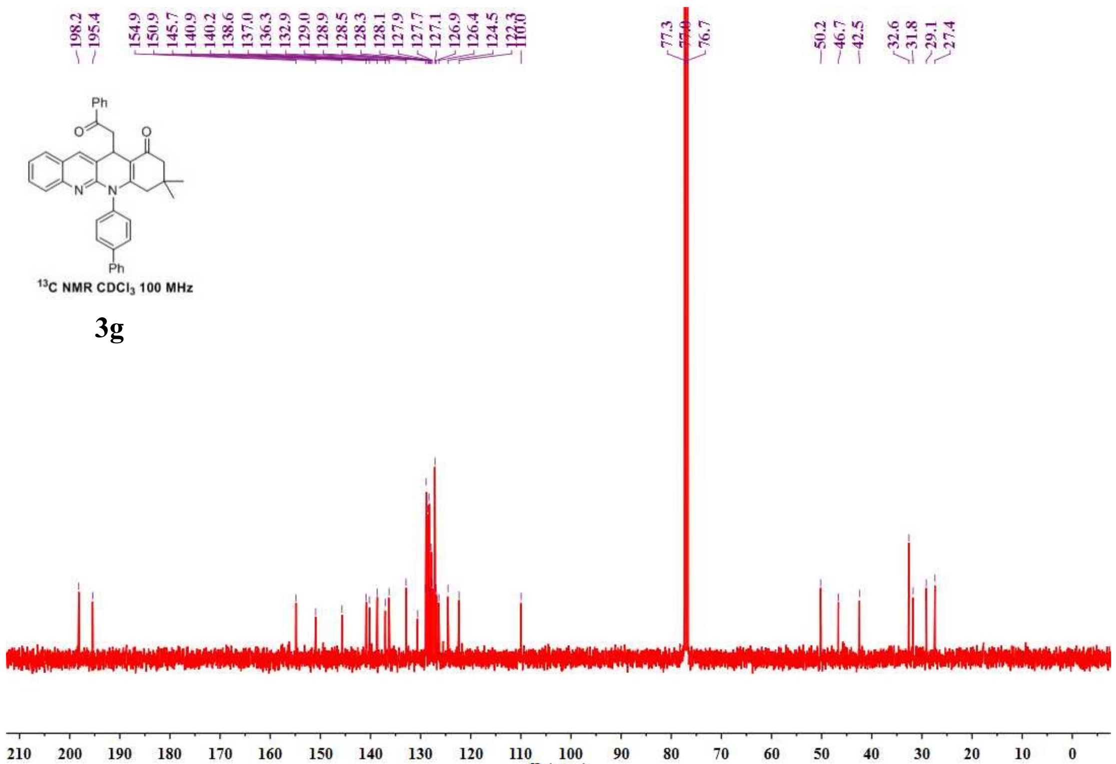
3e


Ph
O
O
N
N
tBu
1H NMR CDCl3 600 MHz
3f
f1 (ppm)

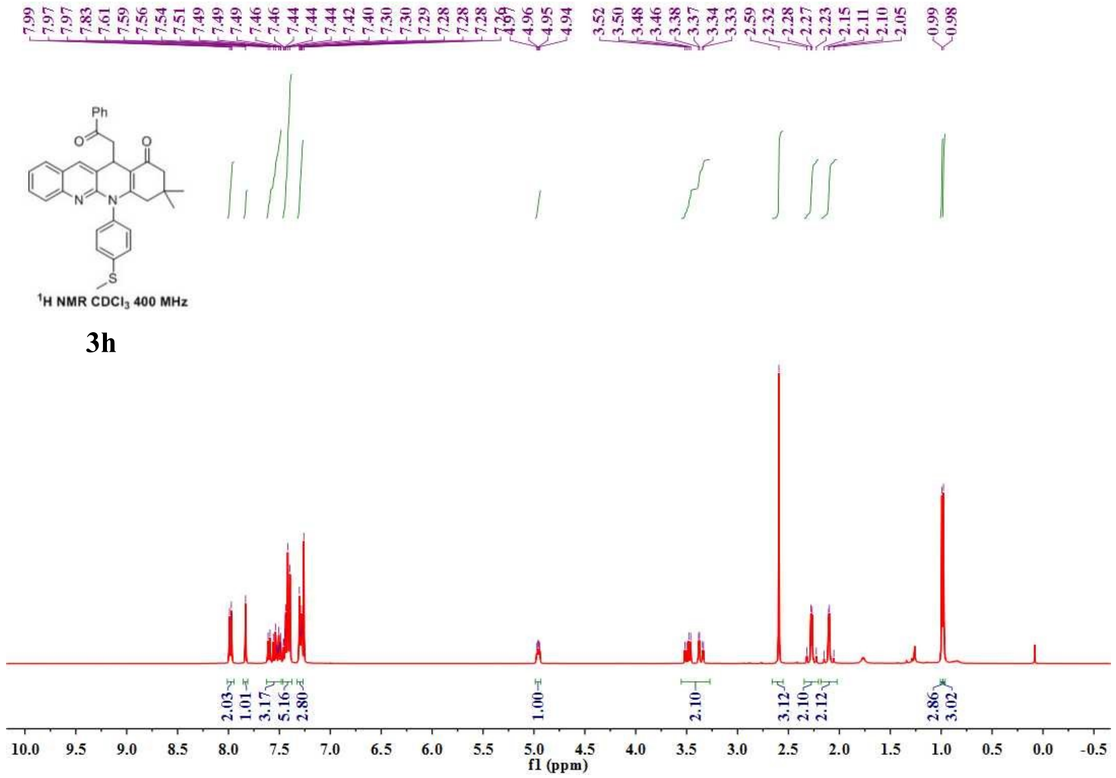

Ph
O
O
N
N
tBu
13C NMR CDCl3 150 MHz
3f
f1 (ppm)



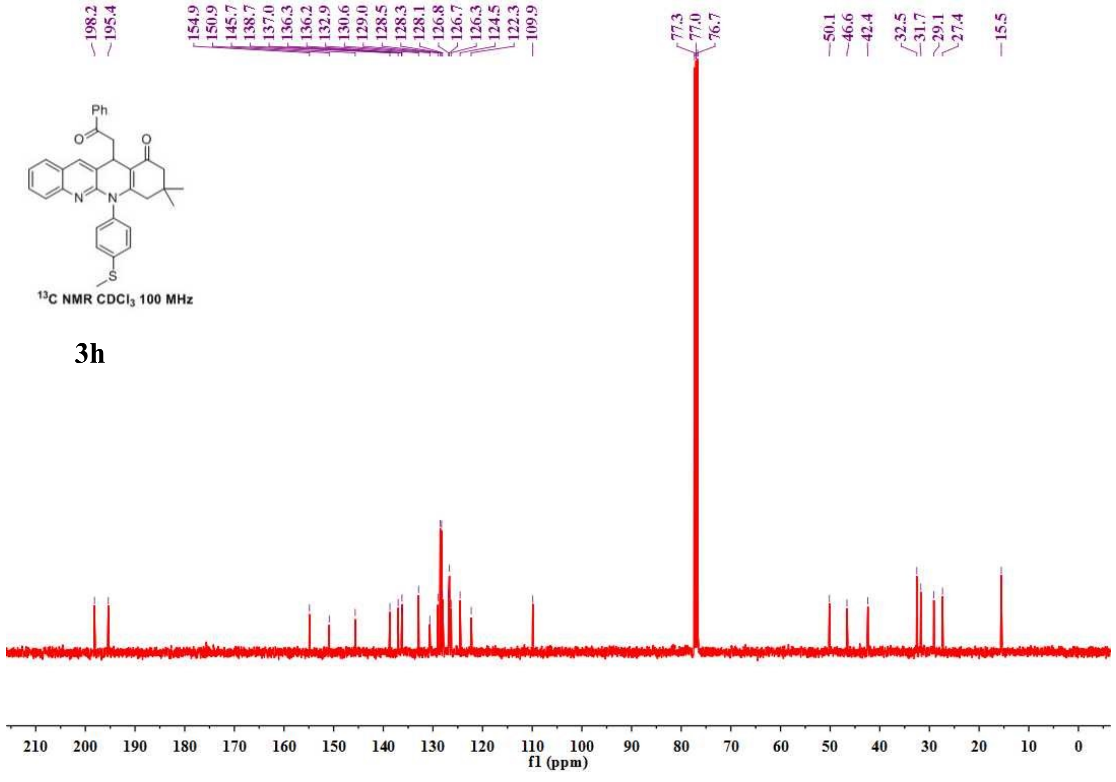
3g



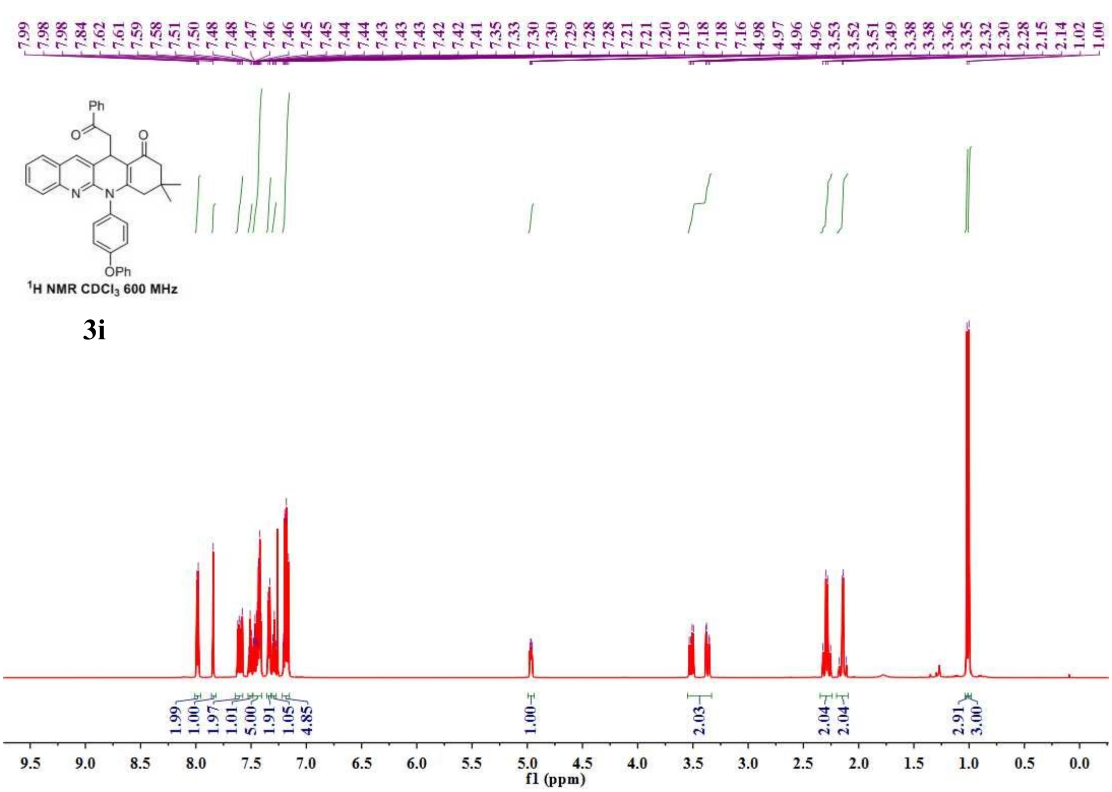
3g


7.99 7.97 7.97 7.83 7.61 7.59 7.56 7.54 7.51 7.49 7.49 7.49 7.46 7.44 7.44 7.44 7.42 7.40 7.30 7.29 7.28 7.28 7.28 7.26 4.97 4.96 4.95 4.94
3.52 3.50 3.48 3.46 3.38 3.37 3.34 3.33 2.59 2.32 2.28 2.27 2.23 2.15 2.11 2.10 2.05 0.99 0.98
Ph
O
N
S
1H NMR CDCl3 400 MHz
2.03 1.01 3.17 5.16 2.80 1.00 2.10 3.12 2.10 2.12 2.86 3.02
f1 (ppm)

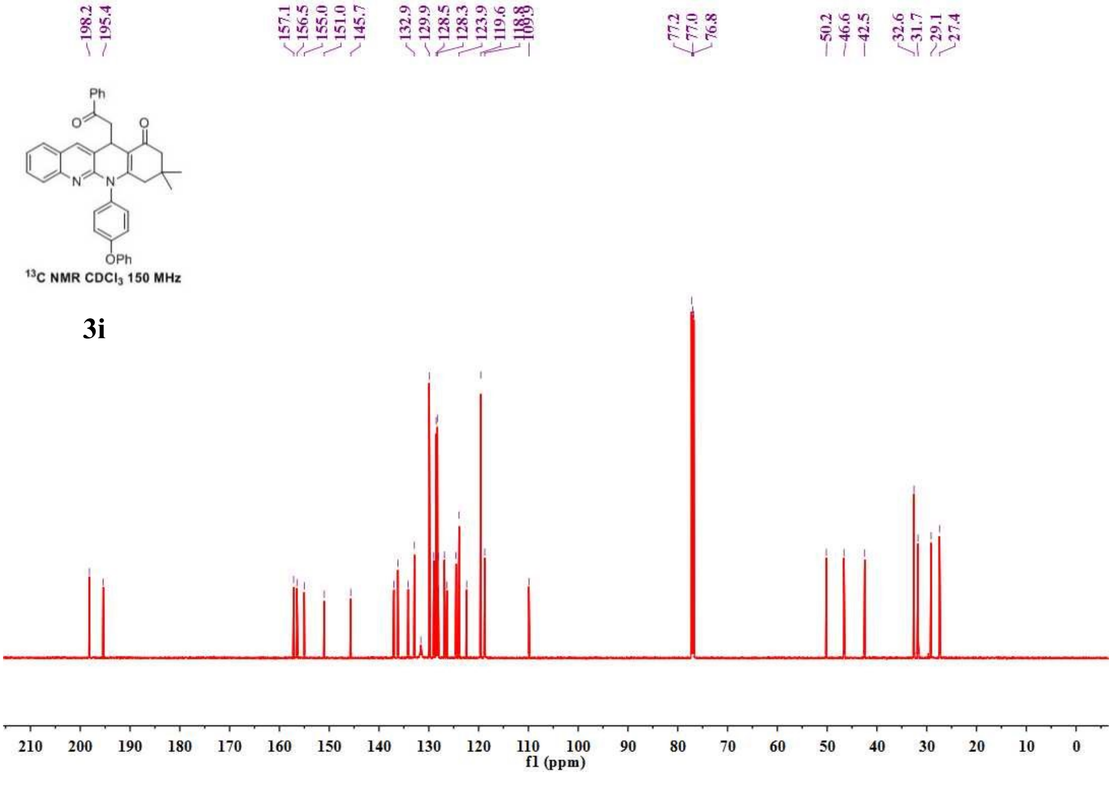
3h


198.2 195.4 154.9 150.9 145.7 138.7 137.0 136.3 136.2 132.9 130.6 129.0 128.5 128.3 128.1 126.8 126.7 126.3 124.5 122.3 109.9 77.3 77.0 76.7 50.1 46.6 42.4 32.5 31.7 29.1 27.4 15.5
Ph
O
N
S
13C NMR CDCl3 100 MHz
f1 (ppm)

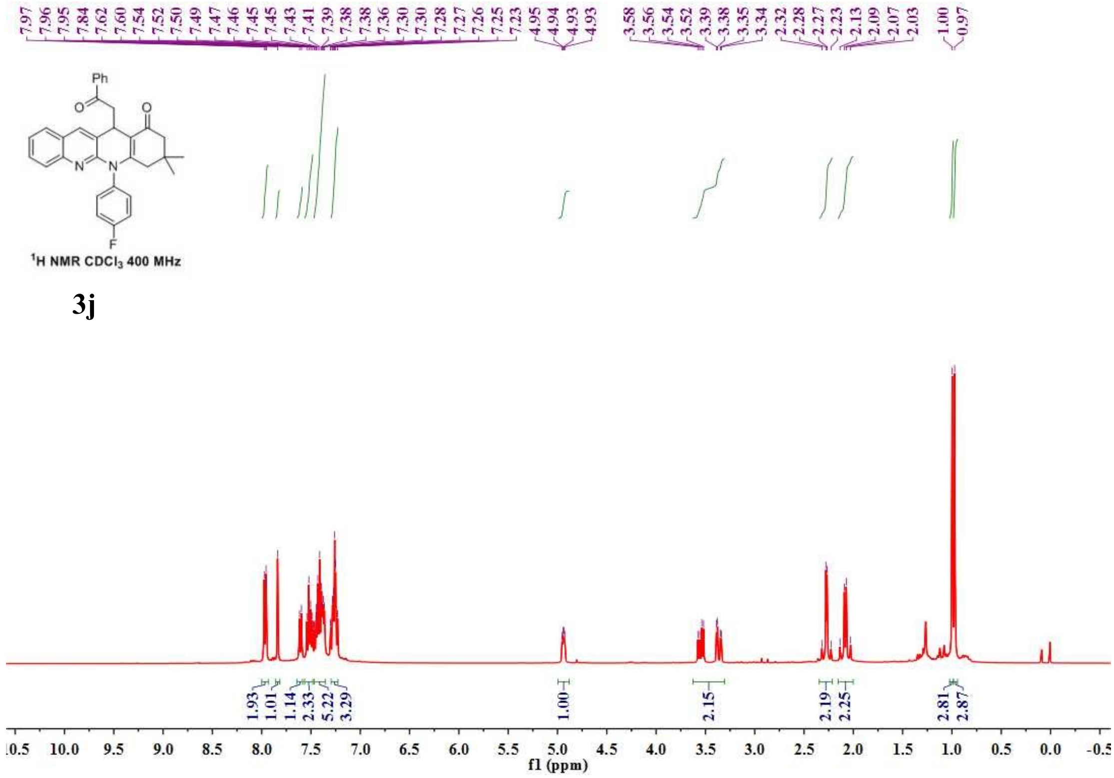
3h



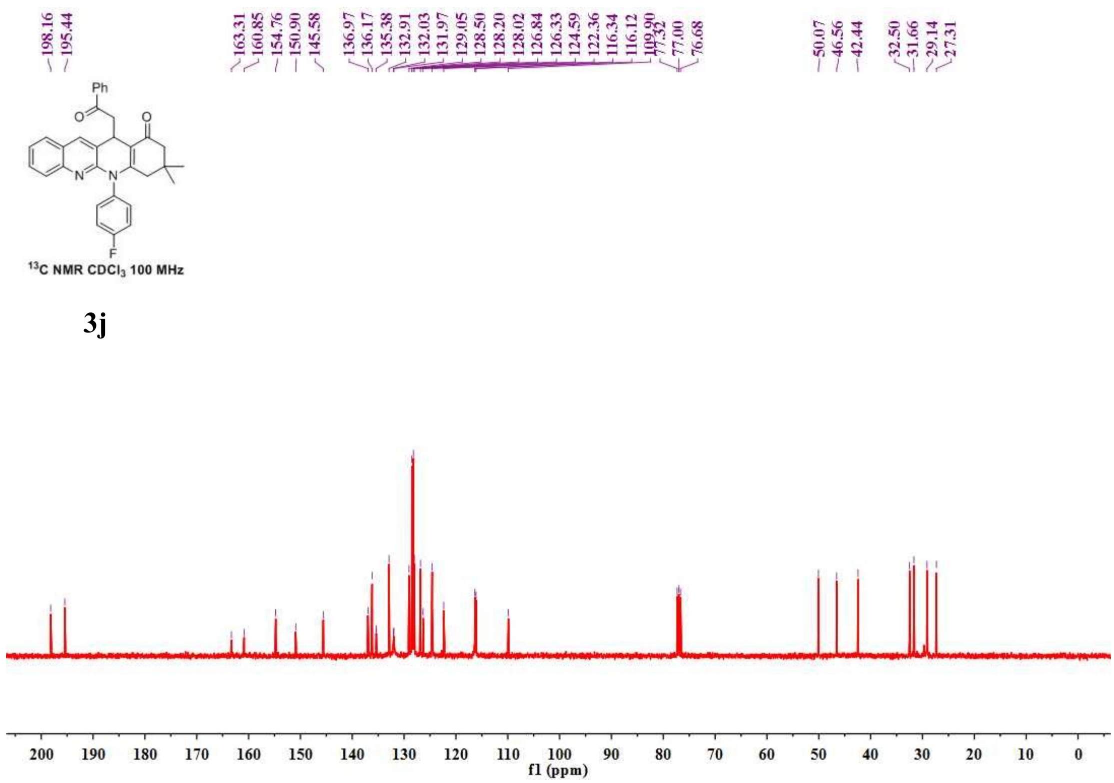
7.99 7.98 7.98 7.84 7.62 7.61 7.59 7.58 7.51 7.50 7.48 7.48 7.47 7.46 7.46 7.45 7.45 7.44 7.44 7.43 7.43 7.43 7.42 7.42 7.41 7.35 7.33 7.30 7.30 7.29 7.28 7.28 7.21 7.21 7.20 7.19 7.18 7.18 7.16 4.98 4.97 4.96 4.96 3.53 3.52 3.51 3.49 3.38 3.38 3.36 3.35 2.32 2.30 2.28 2.15 2.14 1.02 1.00
Ph
O
O
N
N
OPh
1H NMR CDCl3 600 MHz
3i
1.99 1.00 1.97 1.01 5.00 1.91 1.05 4.85 1.00 2.03 2.04 2.04 2.91 3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



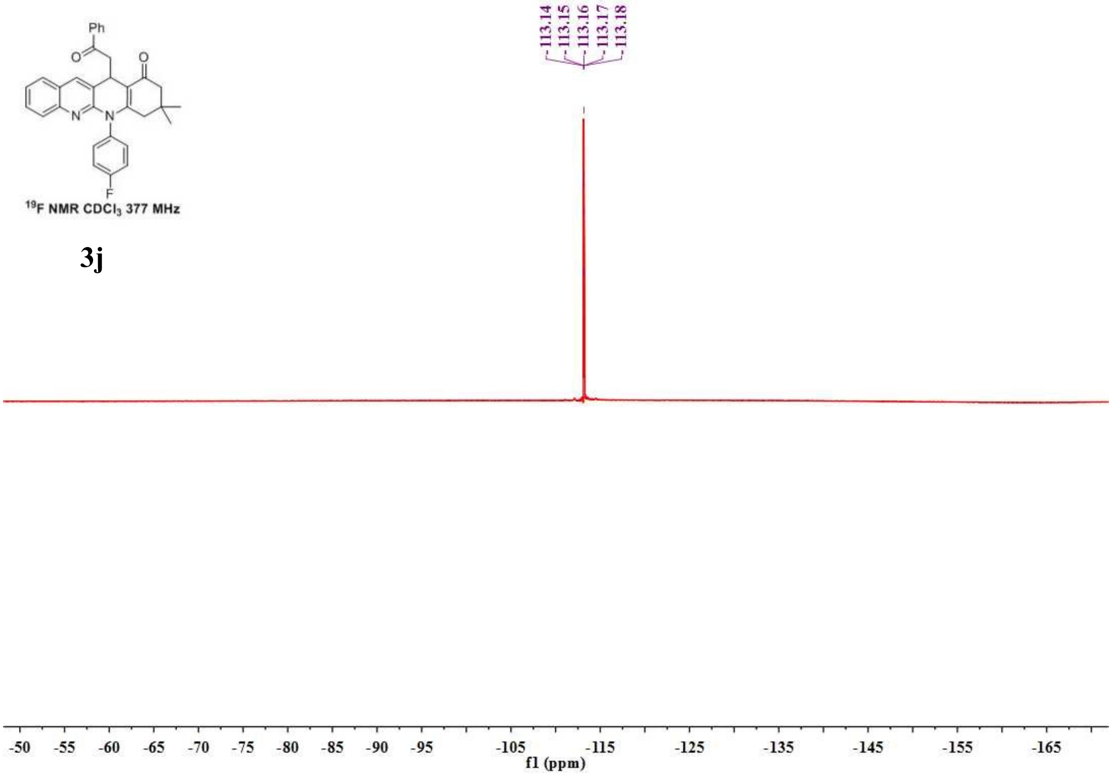
198.2 195.4 157.1 156.5 155.0 151.0 145.7 132.9 129.9 128.5 128.3 123.9 119.6 118.8 109.9 77.2 77.0 76.8 50.2 46.6 42.5 32.6 31.7 29.1 27.4
Ph
O
O
N
N
OPh
13C NMR CDCl3 150 MHz
3i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



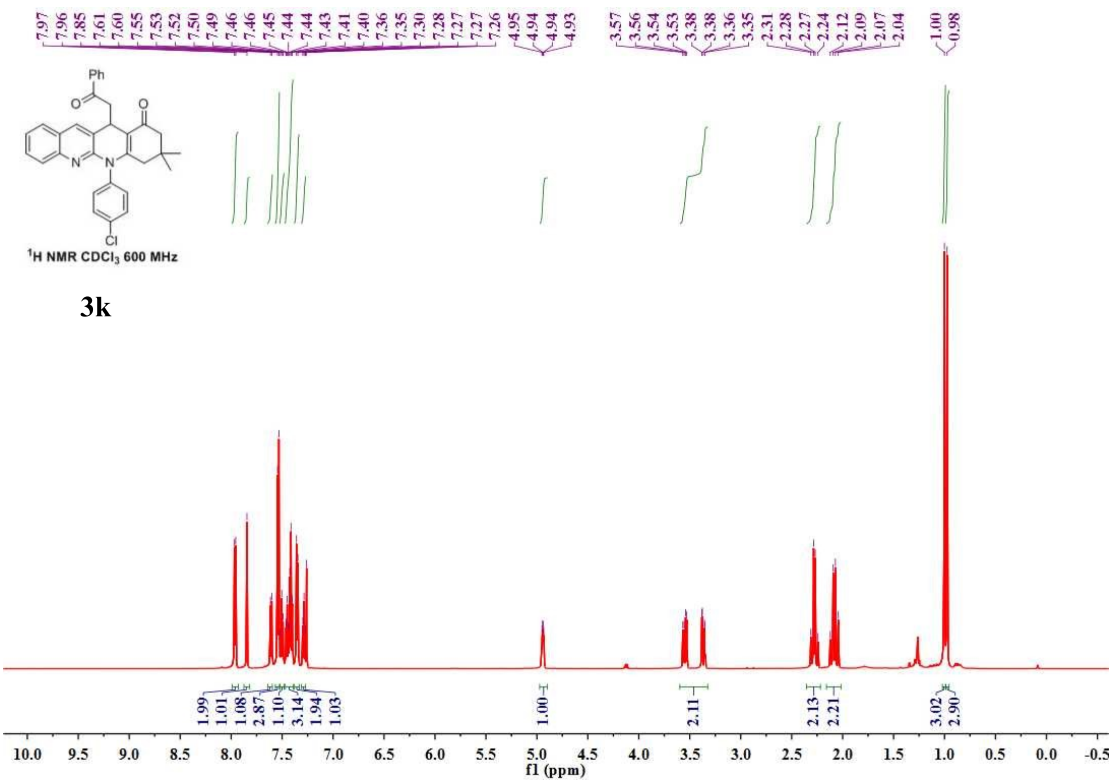
3j



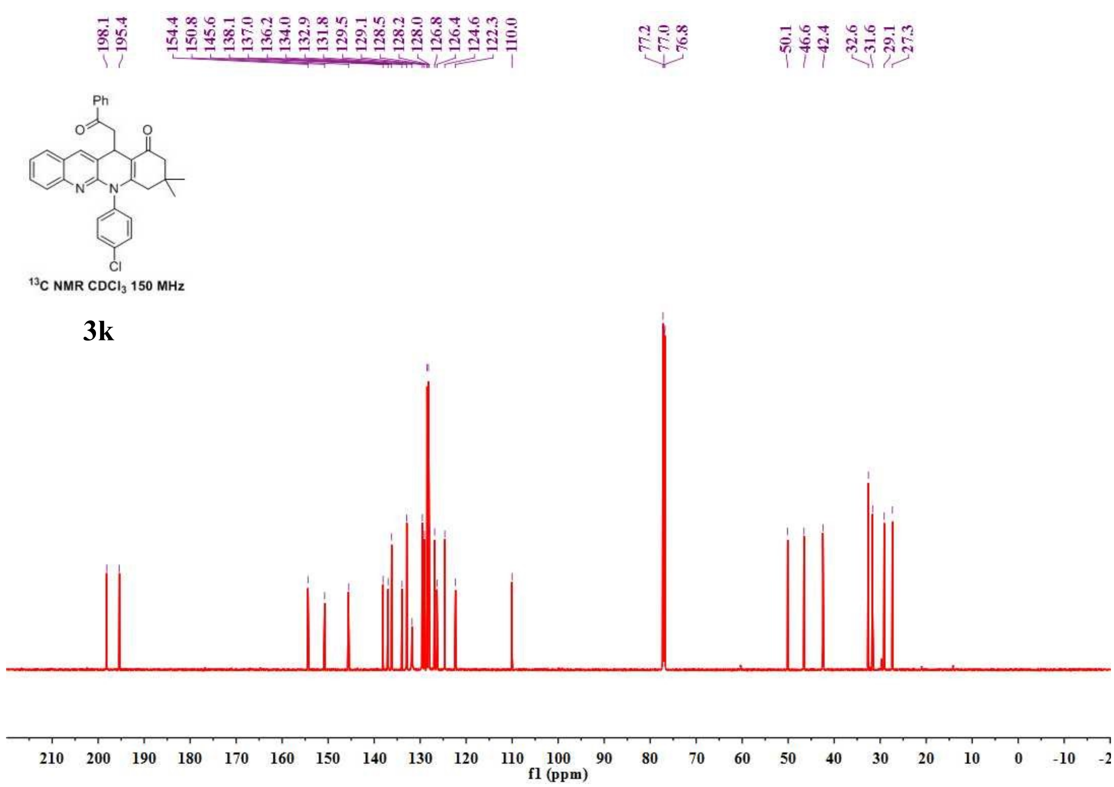
3j


-113.14
-113.15
-113.16
-113.17
-113.18
-50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -105 -115 -125 -135 -145 -155 -165
f1 (ppm)

3j

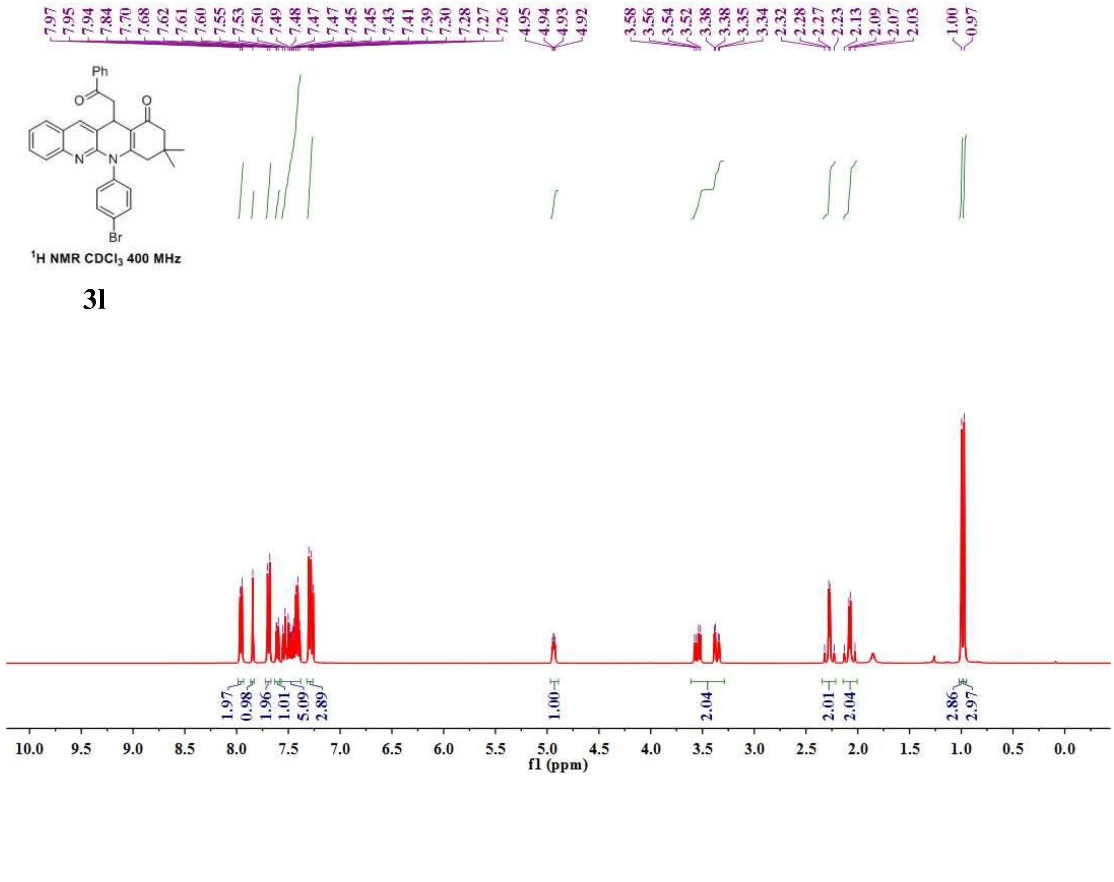

7.97 7.96 7.85 7.61 7.60 7.55 7.53 7.52 7.50 7.49 7.46 7.45 7.44 7.44 7.43 7.41 7.40 7.36 7.35 7.30 7.28 7.27 7.27 7.26 4.95 4.94 4.94 4.93 3.57 3.56 3.54 3.53 3.38 3.38 3.36 3.35 2.31 2.28 2.27 2.24 2.12 2.09 2.07 2.04 1.00 0.98
1.99 1.01 1.08 2.87 1.10 3.14 1.94 1.03 1.00 2.11 2.13 2.21 3.02 2.90
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3k



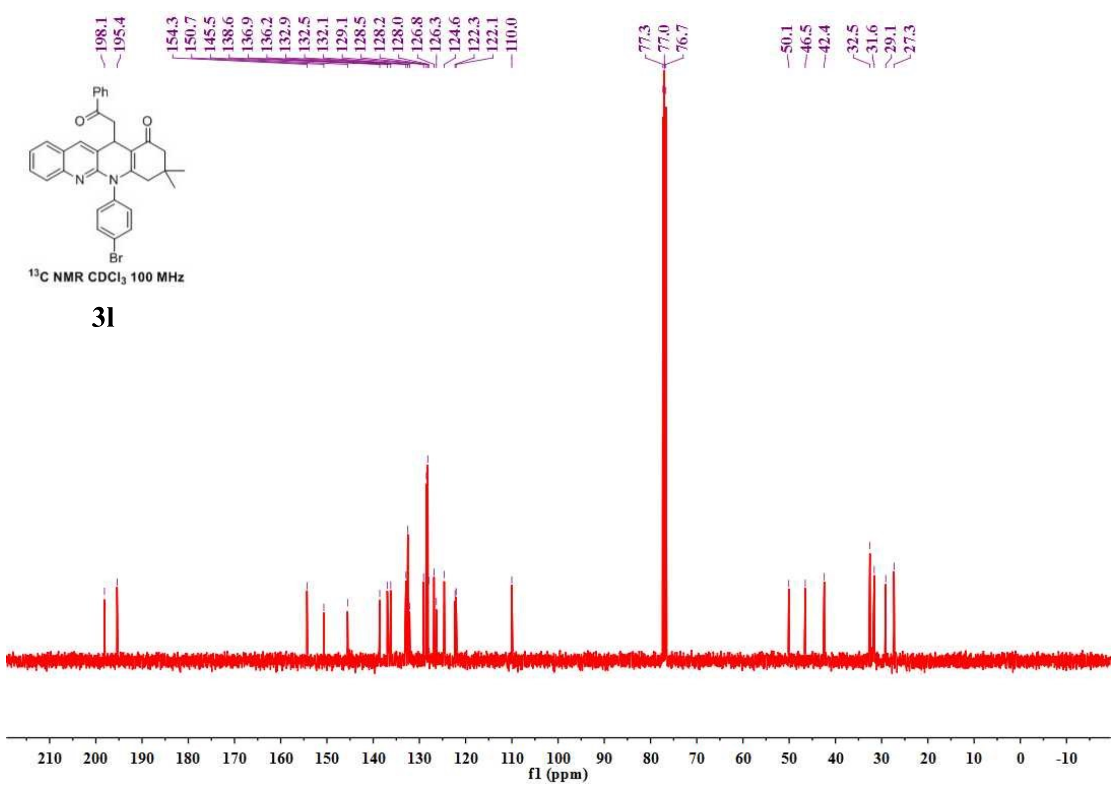
198.1
195.4
154.4
150.8
145.6
138.1
137.0
136.2
134.0
132.9
131.8
129.5
129.1
128.5
128.2
128.0
126.8
126.4
124.6
122.3
110.0
77.2
77.0
76.8
50.1
46.6
42.4
32.6
31.6
29.1
27.3
Ph
O
O
N
N
Cl
13C NMR CDCl3 150 MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3k



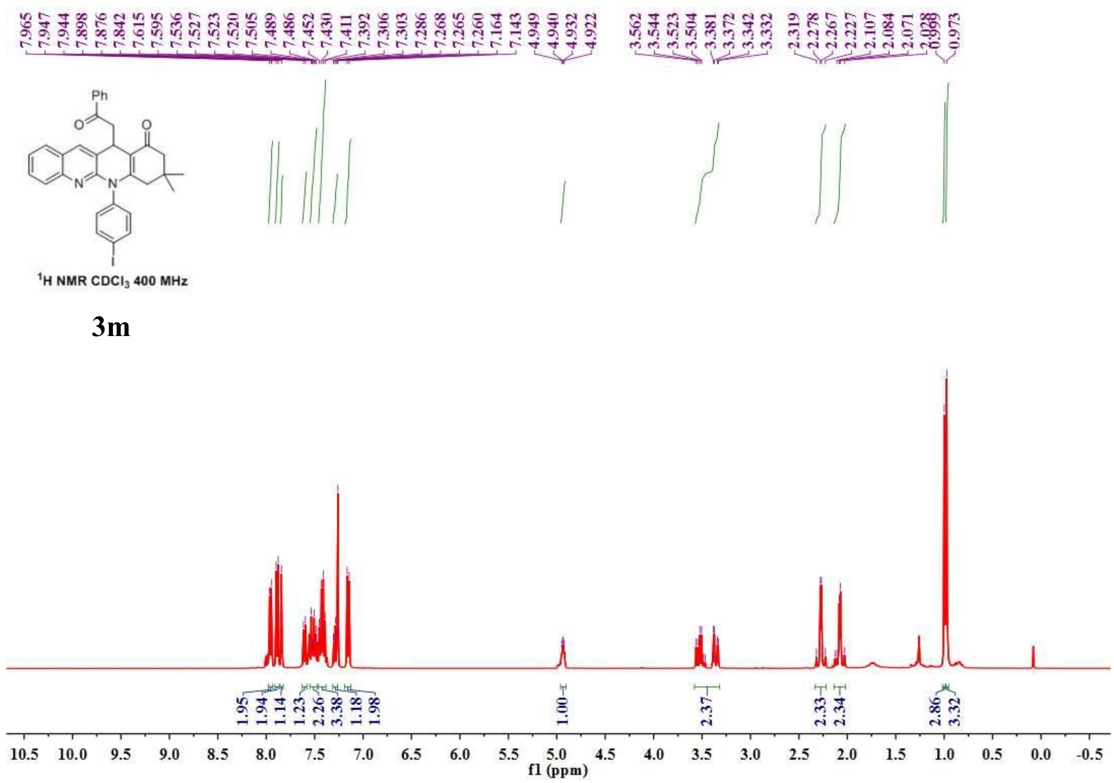
7.97
7.95
7.94
7.84
7.70
7.68
7.62
7.61
7.60
7.55
7.53
7.50
7.49
7.48
7.47
7.45
7.45
7.43
7.41
7.39
7.30
7.28
7.27
7.26
4.95
4.94
4.93
4.92
3.58
3.56
3.54
3.52
3.38
3.38
3.35
3.34
2.32
2.28
2.27
2.23
2.13
2.09
2.07
2.03
1.00
0.97
Ph
O
O
N
N
Br
1H NMR CDCl3 400 MHz
1.97
0.98
1.96
1.01
5.09
2.89
1.00
2.04
2.01
2.04
2.86
2.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3l



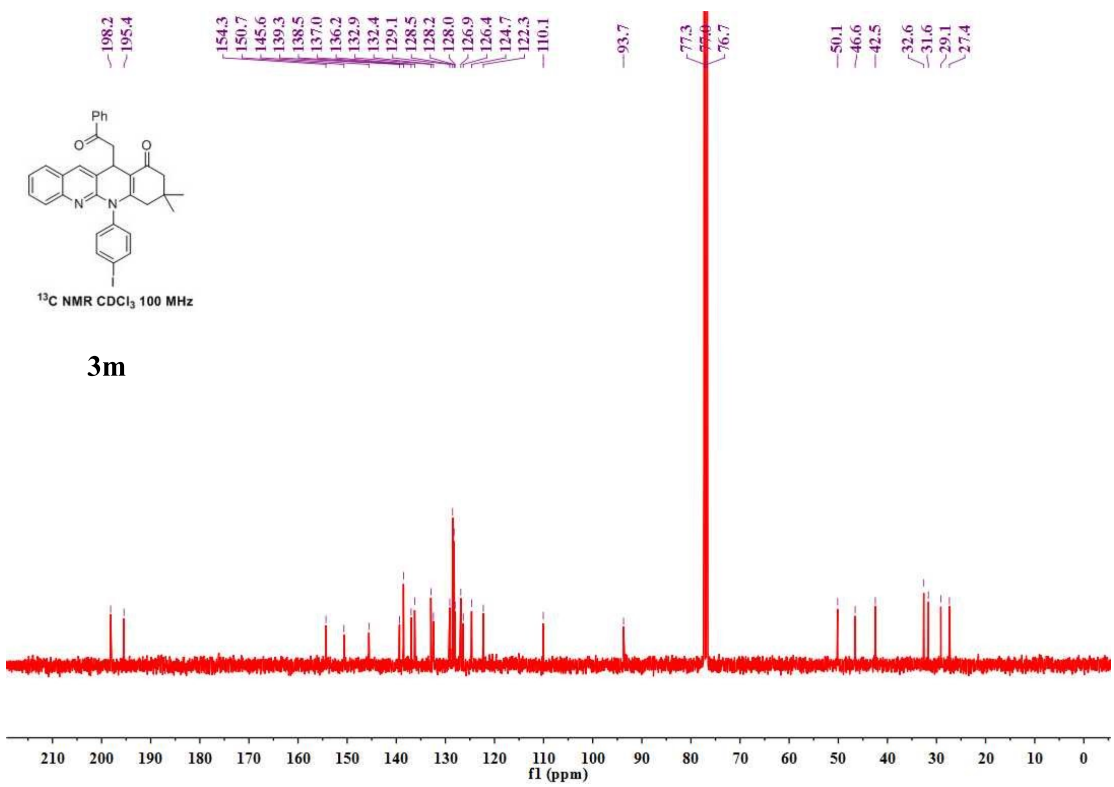
Ph
O
O
N
N
Br
^{13}C NMR CDCl$_3$ 100 MHz
f1 (ppm)

3l

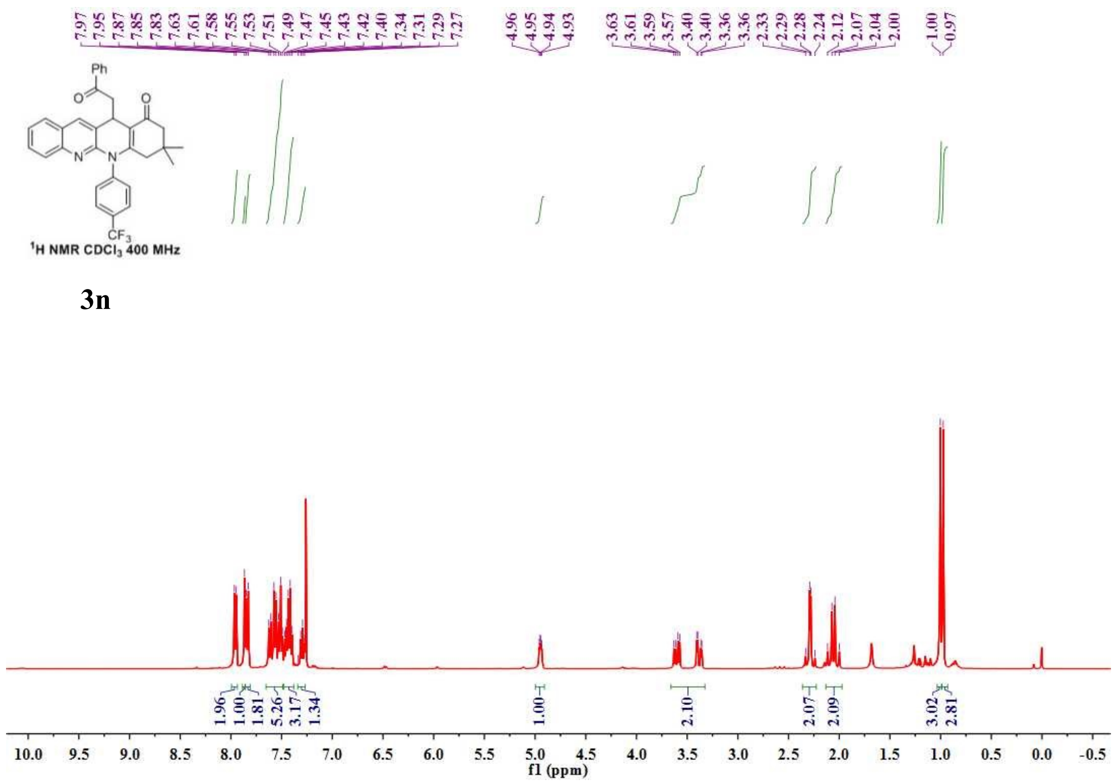


Ph
O
O
N
N
I
^{1}H NMR CDCl$_3$ 400 MHz
f1 (ppm)

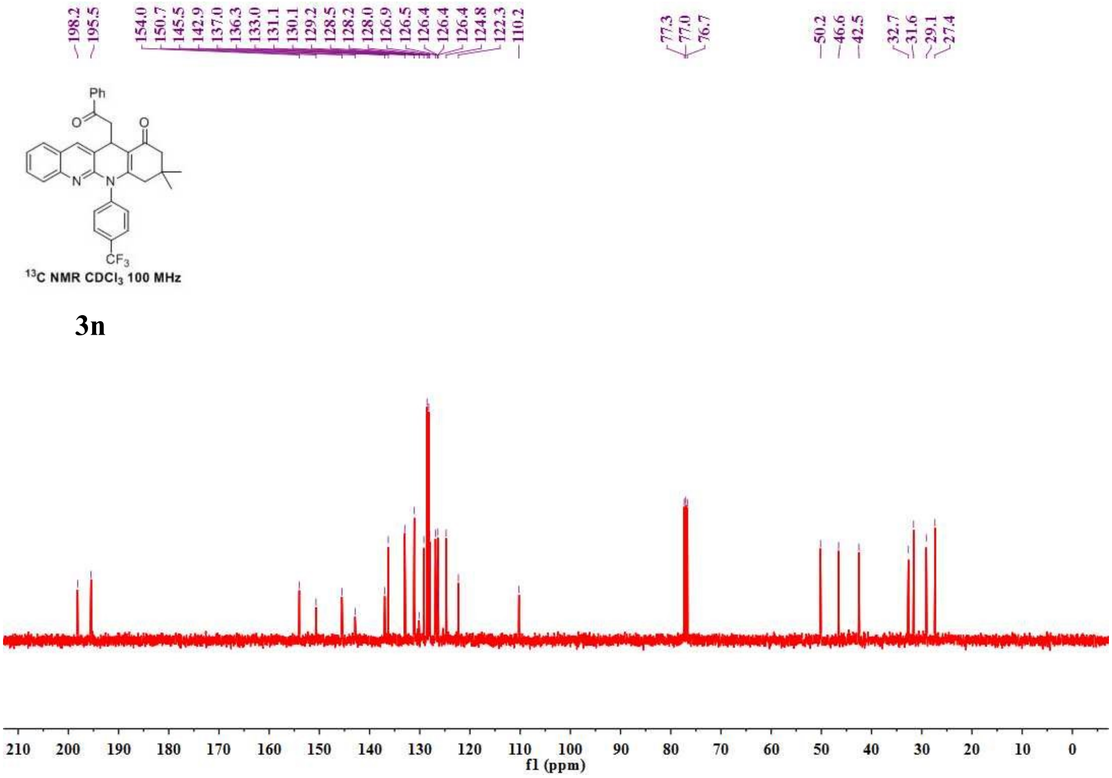
3m


Ph
O
O
N
N
I
13C NMR CDCl3 100 MHz
198.2
195.4
154.3
150.7
145.6
139.3
138.5
137.0
136.2
132.9
132.4
129.1
128.5
128.2
128.0
126.9
126.4
124.7
122.3
110.1
93.7
77.3
77.0
76.7
50.1
46.6
42.5
32.6
31.6
29.1
27.4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

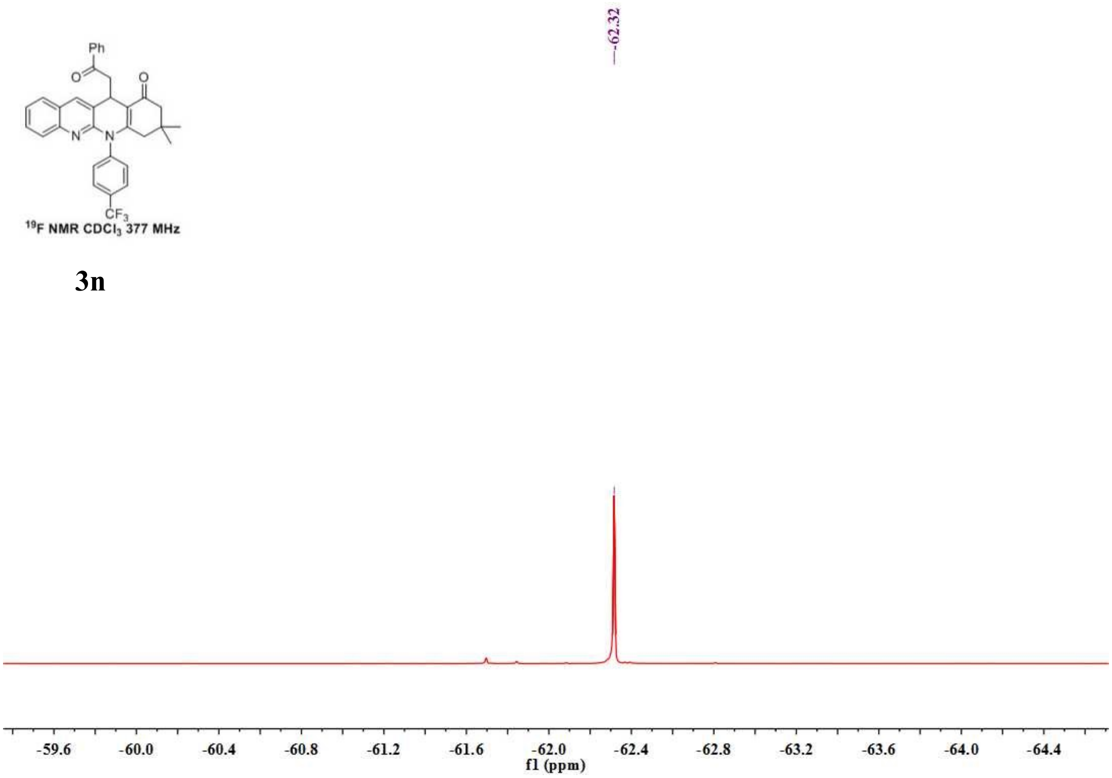
3m


Ph
O
O
N
N
CF3
1H NMR CDCl3 400 MHz
7.97
7.95
7.87
7.85
7.83
7.63
7.61
7.58
7.55
7.53
7.51
7.49
7.47
7.45
7.43
7.42
7.40
7.34
7.31
7.29
7.27
4.96
4.95
4.94
4.93
3.63
3.61
3.59
3.57
3.40
3.40
3.36
2.33
2.29
2.28
2.24
2.12
2.07
2.04
2.00
1.00
0.97
1.96
1.00
1.81
5.26
3.17
1.34
1.00
2.10
2.07
2.09
3.02
2.81
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3n


198.2
195.5
154.0
150.7
145.5
142.9
137.0
136.3
133.0
131.1
130.1
129.2
128.5
128.2
128.0
126.9
126.5
126.4
126.4
126.4
124.8
122.3
110.2
77.3
77.0
76.7
50.2
46.6
42.5
32.7
31.6
29.1
27.4
Ph
O
O
N
N
CF3
13C NMR CDCl3 100 MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3n


-62.32
Ph
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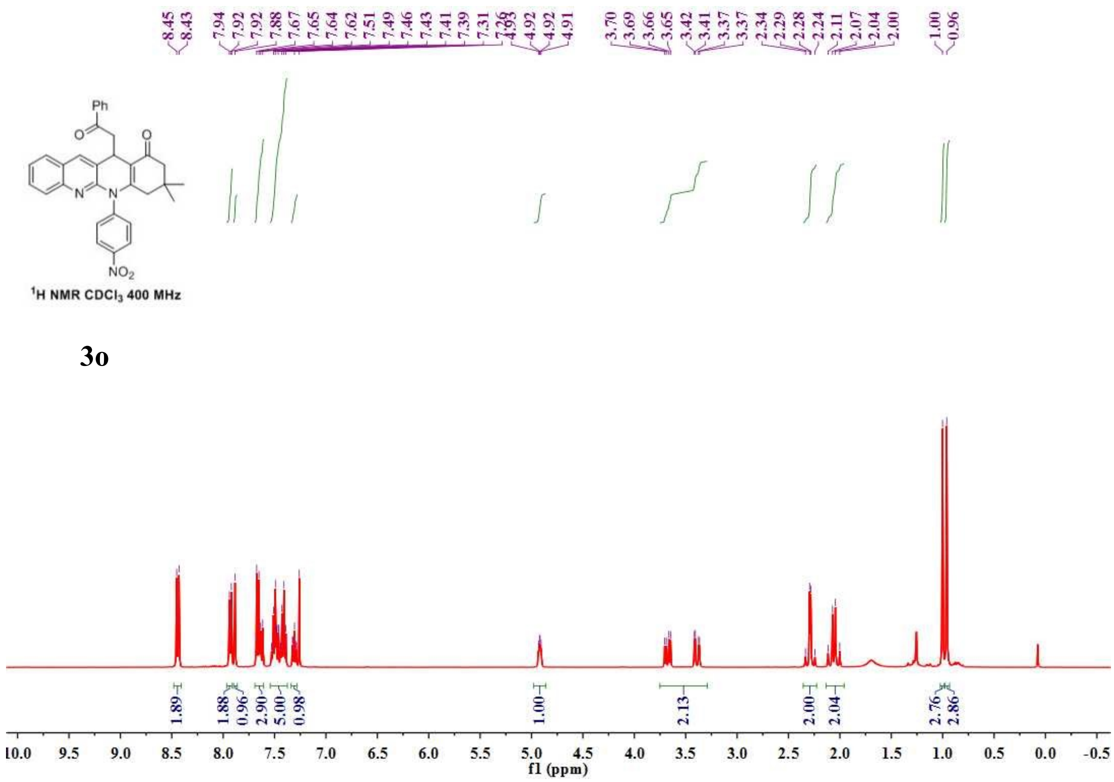
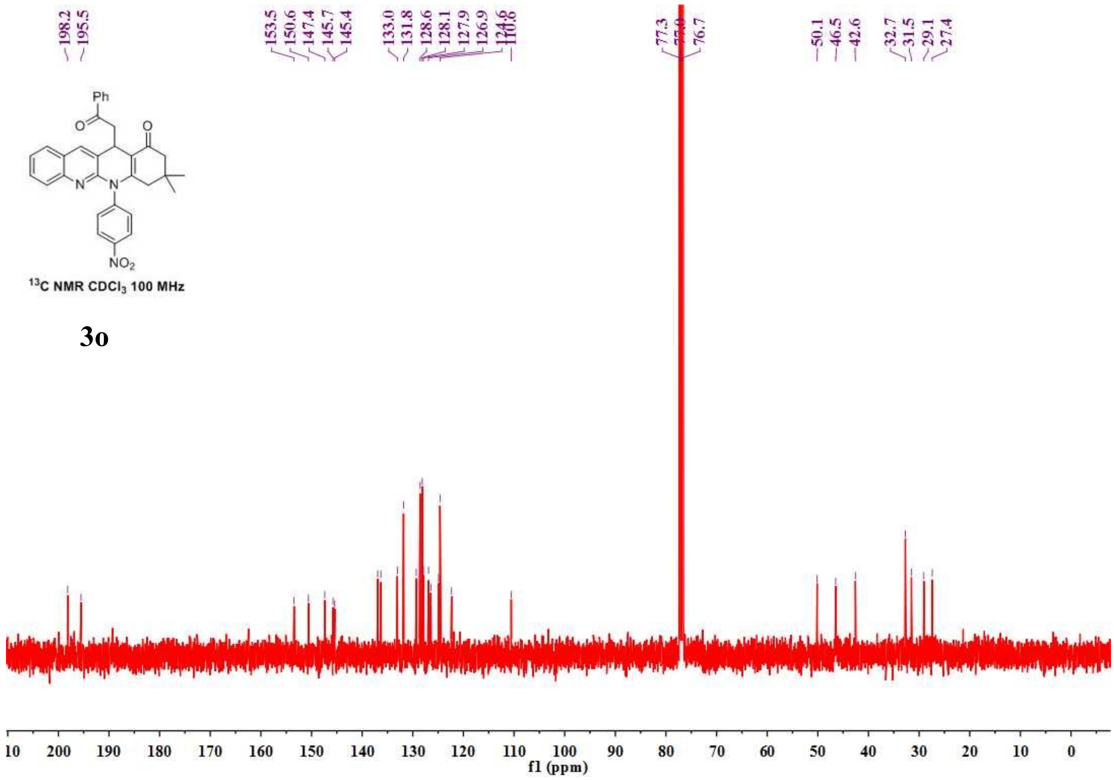
O
N
N
CF3
19F NMR CDCl3 377 MHz
-59.6 -60.0 -60.4 -60.8 -61.2 -61.6 -62.0 -62.4 -62.8 -63.2 -63.6 -64.0 -64.4
f1 (ppm)

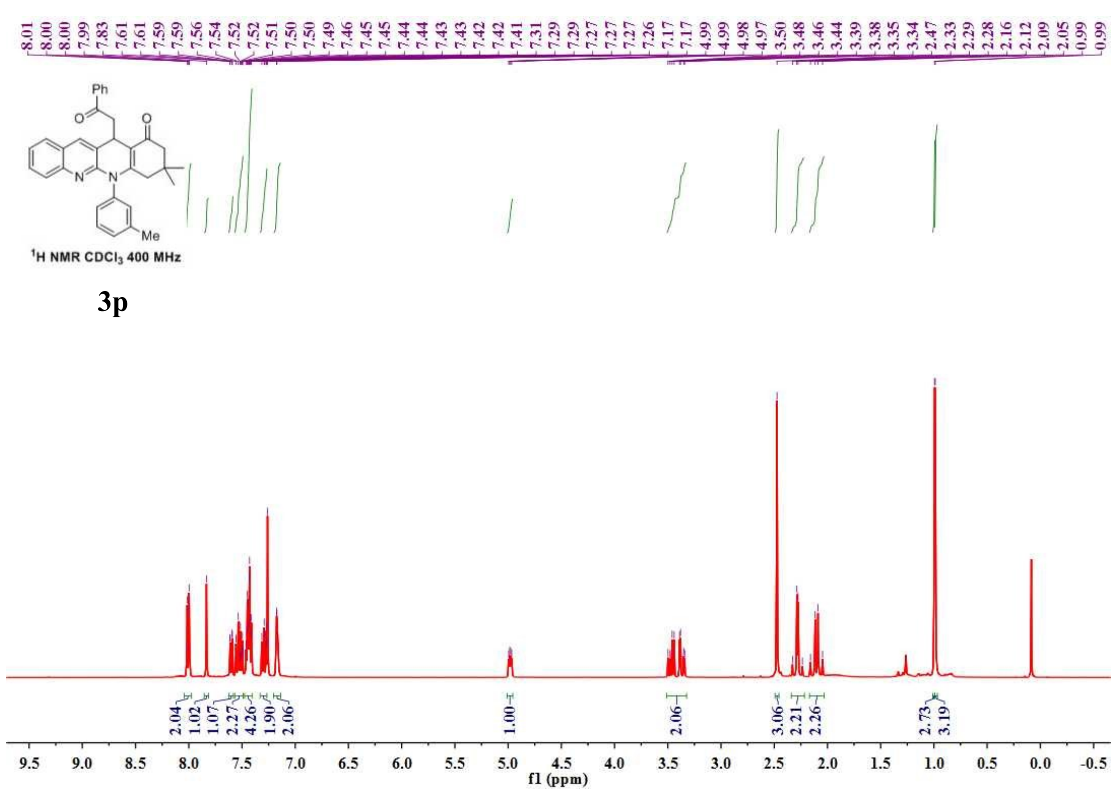
3n


Ph
O
O
N
N
NO_2
^{1}H NMR $CDCl_3$ 400 MHz
f1 (ppm)

3o

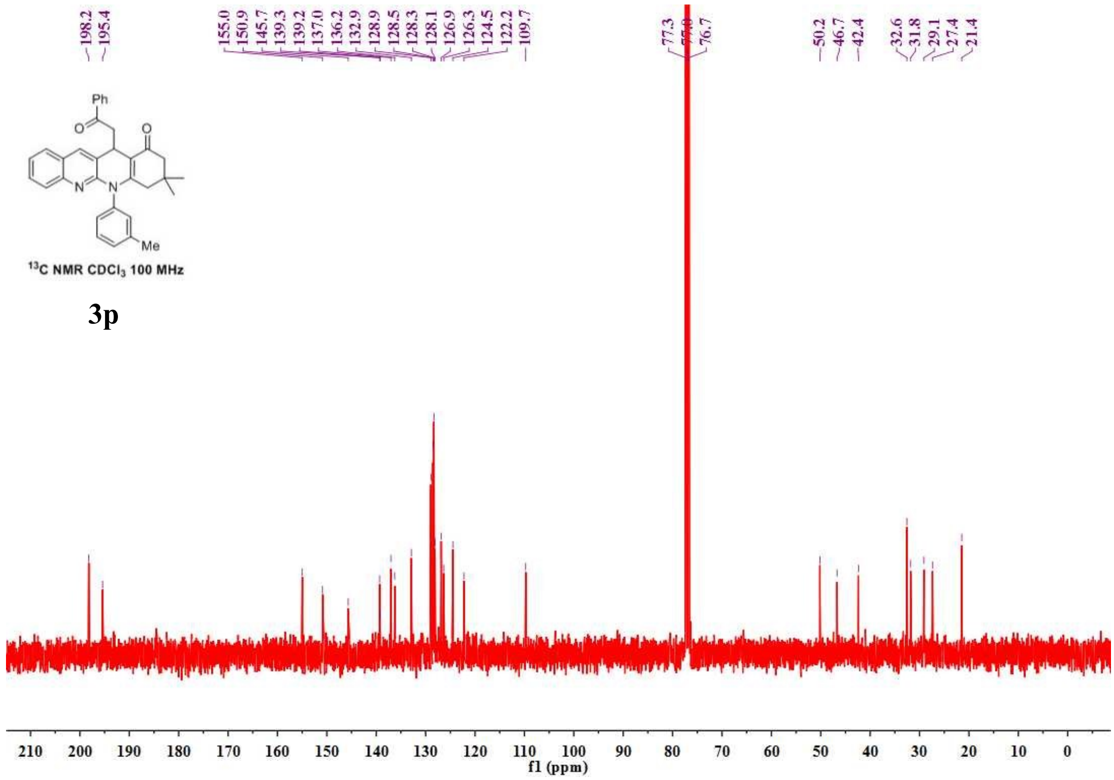

Ph
O
O
N
N
NO_2
^{13}C NMR $CDCl_3$ 100 MHz
f1 (ppm)

3o



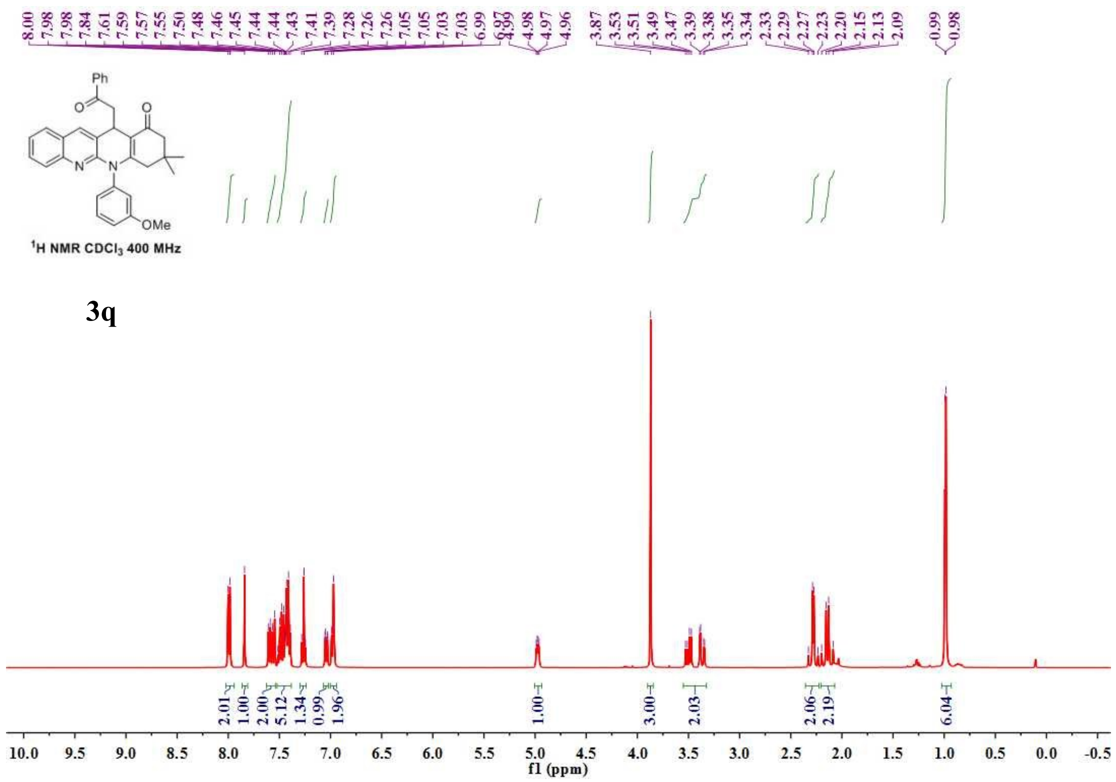
8.01 8.00 8.00 7.99 7.83 7.61 7.61 7.59 7.59 7.56 7.54 7.52 7.52 7.51 7.50 7.50 7.49 7.46 7.45 7.45 7.44 7.44 7.43 7.43 7.42 7.42 7.41 7.31 7.29 7.29 7.27 7.27 7.27 7.26 7.17 7.17 4.99 4.99 4.98 4.97 3.50 3.48 3.46 3.44 3.39 3.38 3.35 3.34 2.47 2.33 2.29 2.28 2.16 2.12 2.09 2.05 0.99 0.99
Ph
O
O
N
N
Me
^{1}H NMR CDCl$_3$ 400 MHz
2.04 1.02 1.07 2.27 4.26 1.90 2.06 1.00 2.06 3.06 2.21 2.26 2.73 3.19
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

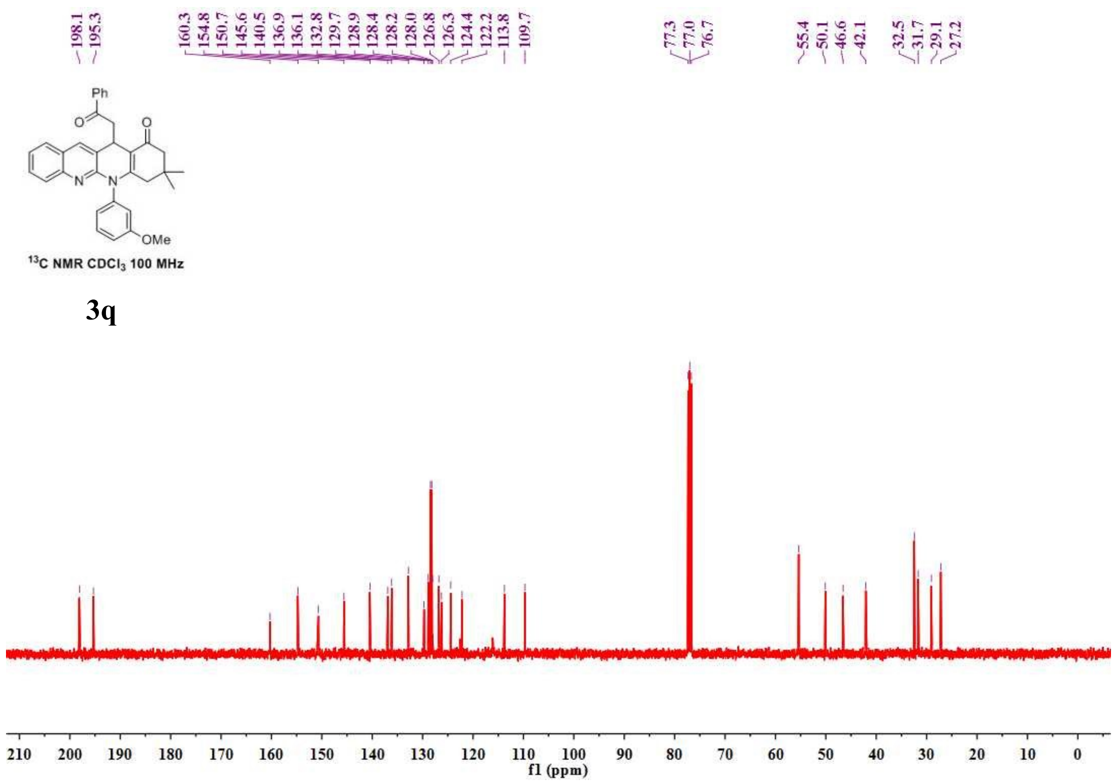
3p

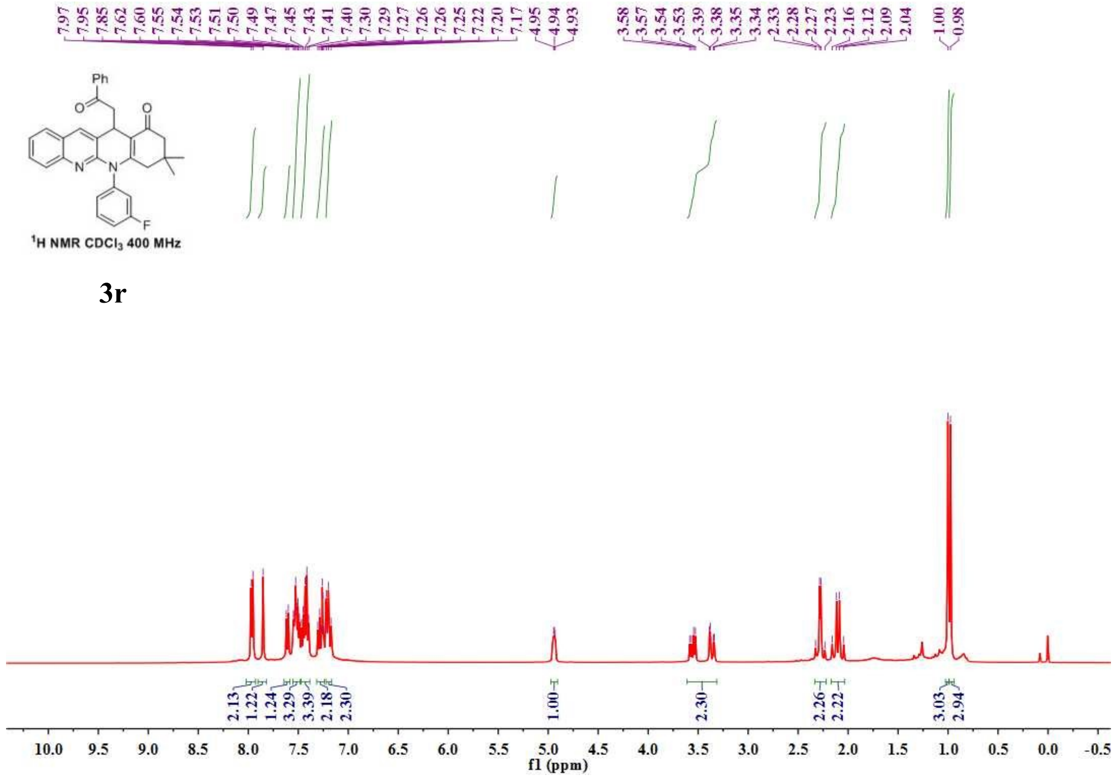


198.2 195.4 155.0 150.9 145.7 139.3 139.2 137.0 136.2 132.9 128.9 128.5 128.3 128.1 126.9 126.3 124.5 122.2 109.7 77.3 77.0 76.7 50.2 46.7 42.4 32.6 31.8 29.1 27.4 21.4
Ph
O
O
N
N
Me
^{13}C NMR CDCl$_3$ 100 MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3p


8.00 7.98 7.98 7.84 7.61 7.59 7.57 7.55 7.50 7.48 7.46 7.45 7.44 7.44 7.43 7.41 7.39 7.28 7.26 7.26 7.05 7.05 7.03 7.03 6.99 6.97 4.99 4.98 4.97 4.96 3.87 3.53 3.51 3.49 3.47 3.39 3.38 3.35 3.34 2.33 2.29 2.27 2.23 2.20 2.15 2.13 2.09 0.99 0.98
Ph
O
N
OMe
1H NMR CDCl3 400 MHz
3q
2.01 1.00 2.00 5.12 1.34 0.99 1.96 1.00 3.00 2.03 2.06 2.19 6.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


198.1 195.3 160.3 154.8 150.7 145.6 140.5 136.9 136.1 132.8 129.7 128.9 128.4 128.2 128.0 126.8 126.3 124.4 122.2 113.8 109.7 77.3 77.0 76.7 55.4 50.1 46.6 42.1 32.5 31.7 29.1 27.2
Ph
O
N
OMe
13C NMR CDCl3 100 MHz
3q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



7.97
7.95
7.85
7.62
7.60
7.55
7.54
7.53
7.51
7.50
7.49
7.47
7.45
7.43
7.41
7.40
7.30
7.29
7.27
7.26
7.26
7.25
7.22
7.20
7.17
4.95
4.94
4.93
3.58
3.57
3.54
3.53
3.39
3.38
3.35
3.34
2.33
2.28
2.27
2.23
2.16
2.12
2.09
2.04
1.00
0.98
Ph
O
O
N
N
F
[1]H NMR CDCl3 400 MHz
2.13
1.22
1.24
3.29
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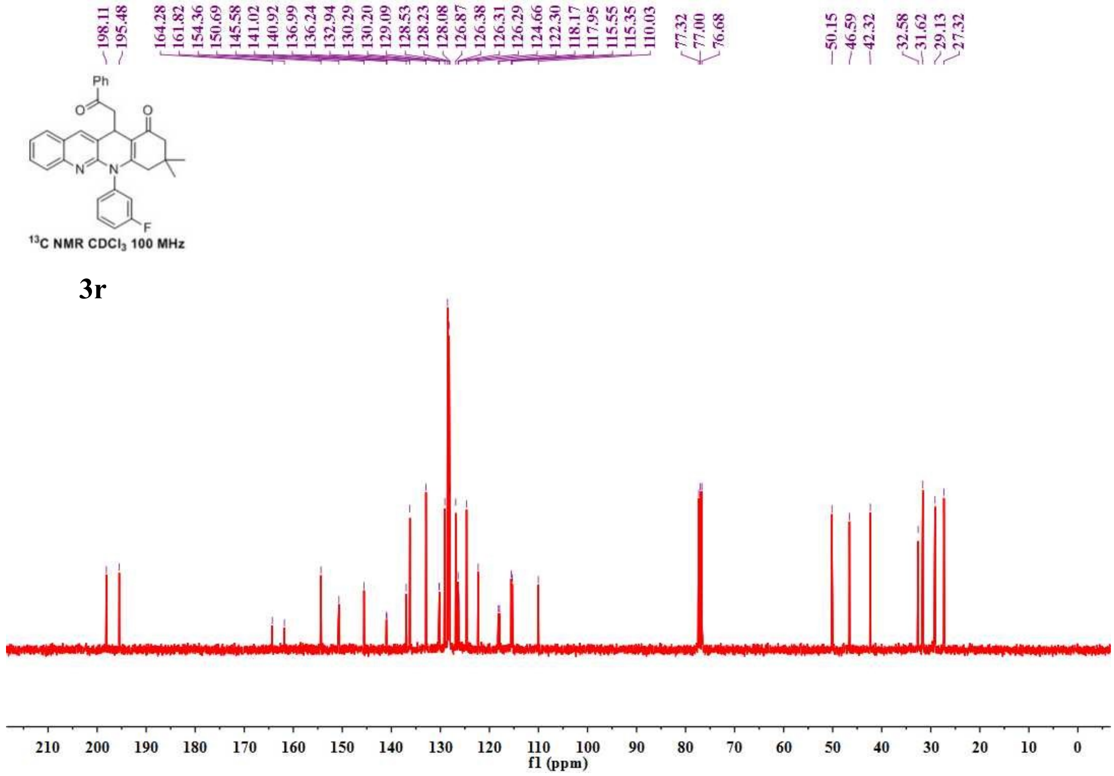
2.18
2.30
1.00
2.30
2.26
2.22
3.03
2.94
f1 (ppm)

3r



198.11
195.48
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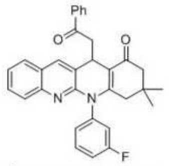
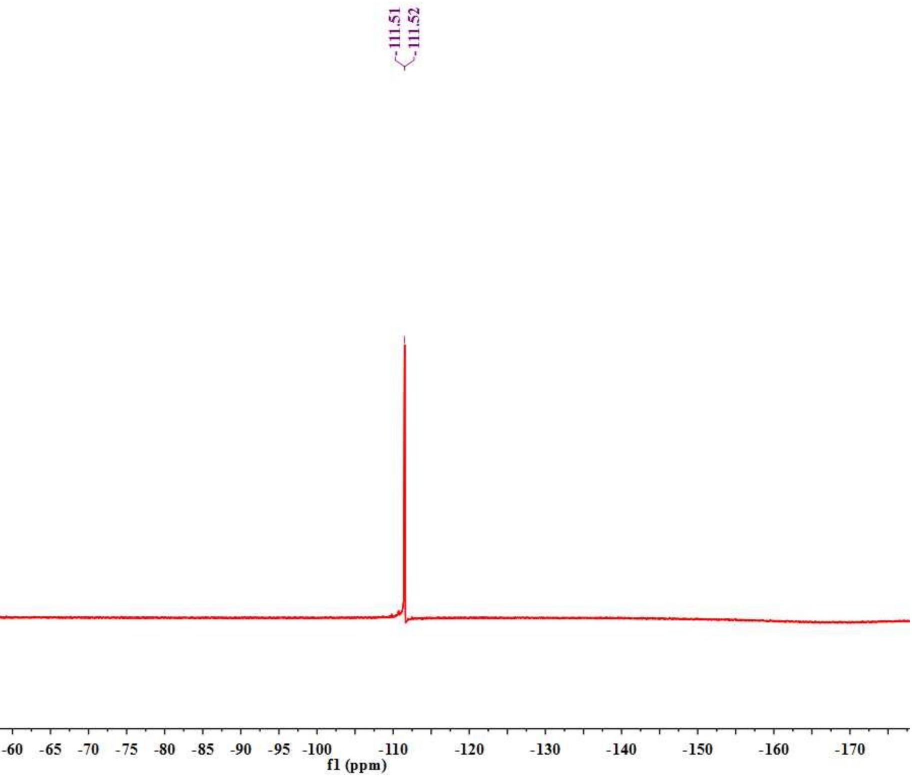
161.82
154.36
150.69
145.58
141.02
140.92
136.99
136.24
132.94
130.29
130.20
129.09
128.53
128.23
128.08
126.87
126.38
126.31
126.29
124.66
122.30
118.17
117.95
115.55
115.35
110.03
77.32
77.00
76.68
50.15
46.59
42.32
32.58
31.62
29.13
27.32
Ph
O
O
N
N
F
[13]C NMR CDCl3 100 MHz
f1 (ppm)

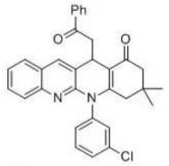
3r



^{19}F NMR CDCl$_3$ 377 MHz

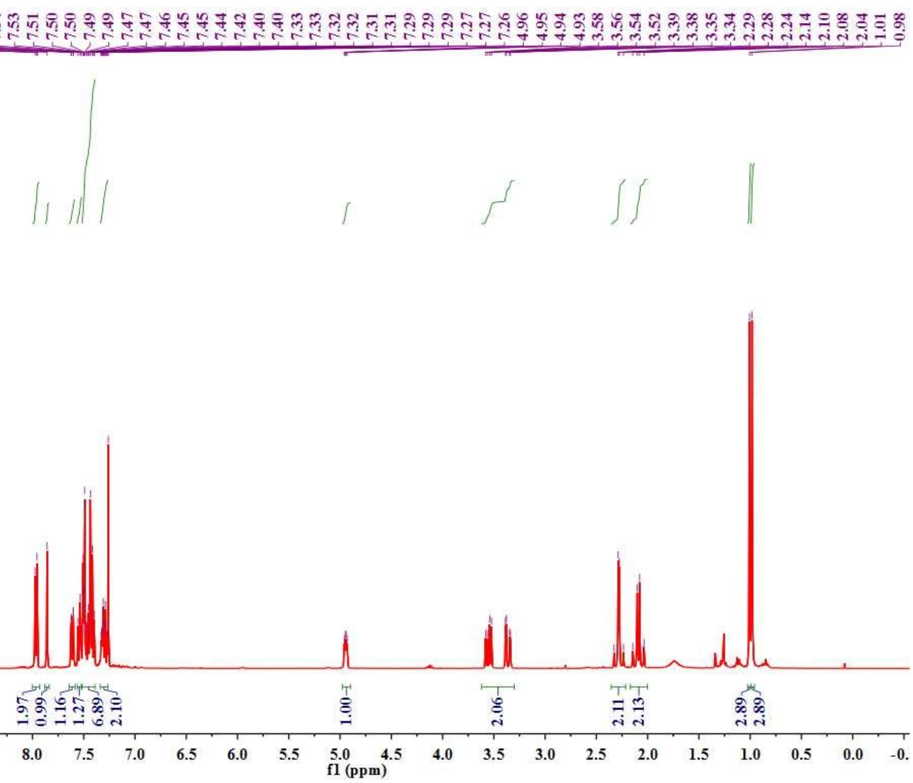
3r

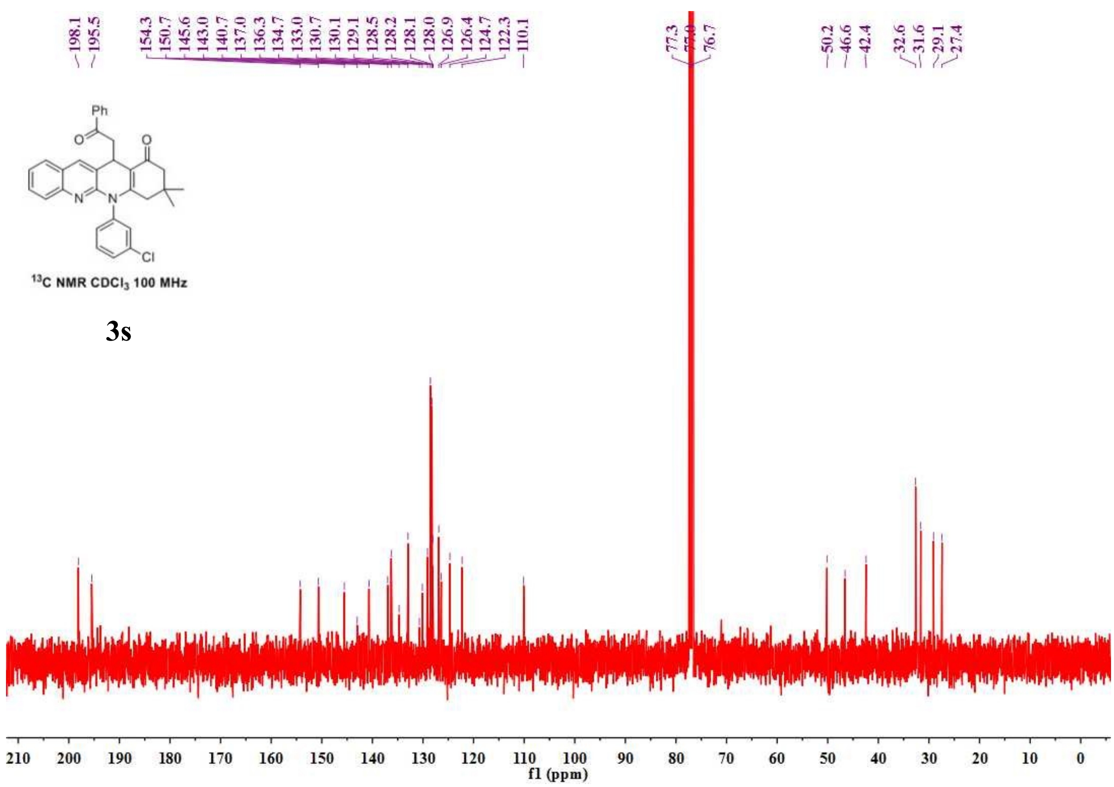




^{1}H NMR CDCl$_3$ 400 MHz

3s

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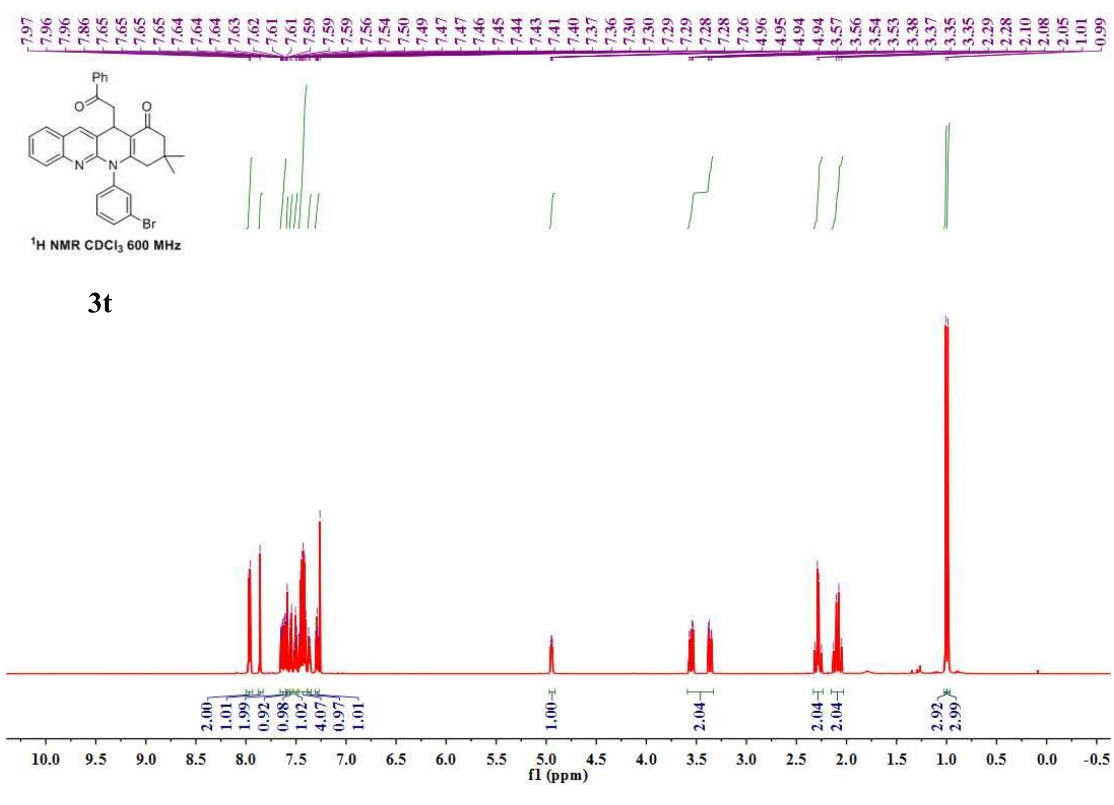
140.7
137.0
136.3
134.7
133.0
130.7
130.1
129.1
128.5
128.2
128.1
128.0
126.9
126.4
124.7
122.3
110.1
77.3
77.0
76.7
50.2
46.6
42.4
32.6
31.6
29.1
27.4
Ph
O
O
N
N
Cl
^{13}C NMR CDCl$_3$ 100 MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3s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7.86
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7.64
7.63
7.62
7.61
7.61
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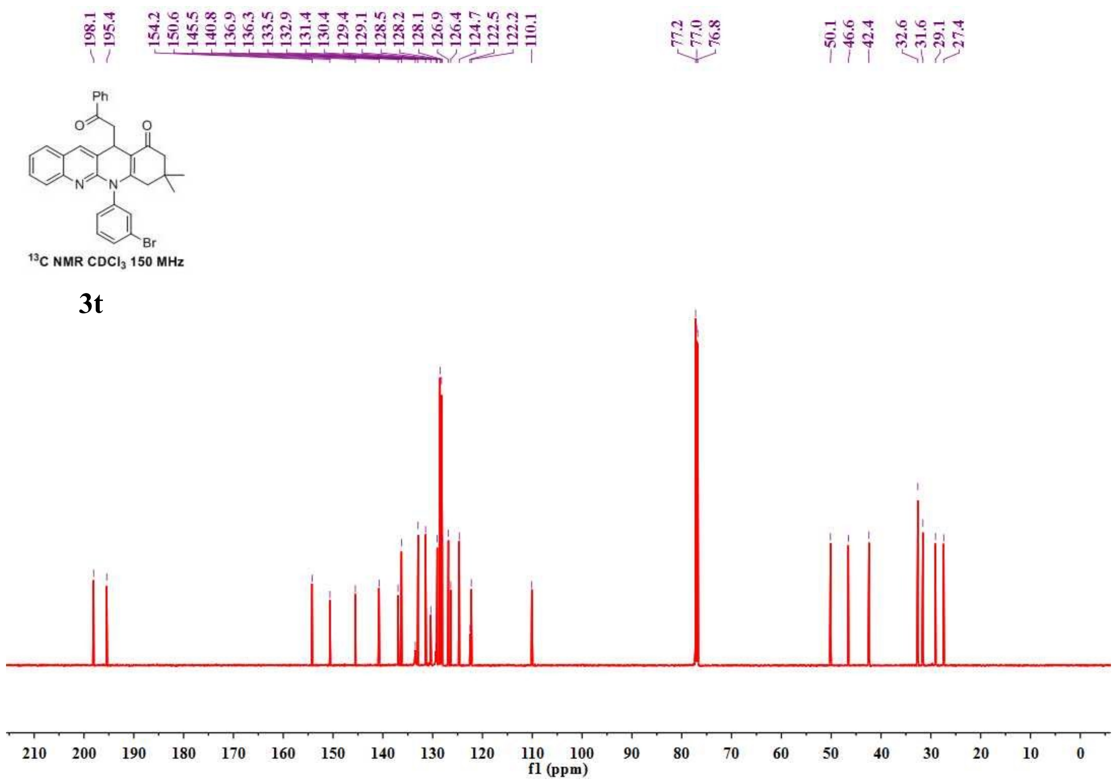
7.59
7.59
7.56
7.54
7.50
7.49
7.47
7.46
7.45
7.44
7.43
7.41
7.40
7.37
7.36
7.30
7.30
7.29
7.29
7.28
7.28
7.26
4.96
4.95
4.94
3.57
3.56
3.54
3.53
3.38
3.37
3.35
3.35
2.29
2.28
2.10
2.08
2.05
1.01
0.99
Ph
O
O
N
N
Br
^{1}H NMR CDCl$_3$ 600 MHz
2.00
1.01
1.99
0.92
0.98
1.02
4.07
0.97
1.01
1.00
2.04
2.04
2.04
2.92
2.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3t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130.4
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129.1
128.5
128.2
128.1
126.9
126.4
124.7
122.5
122.2
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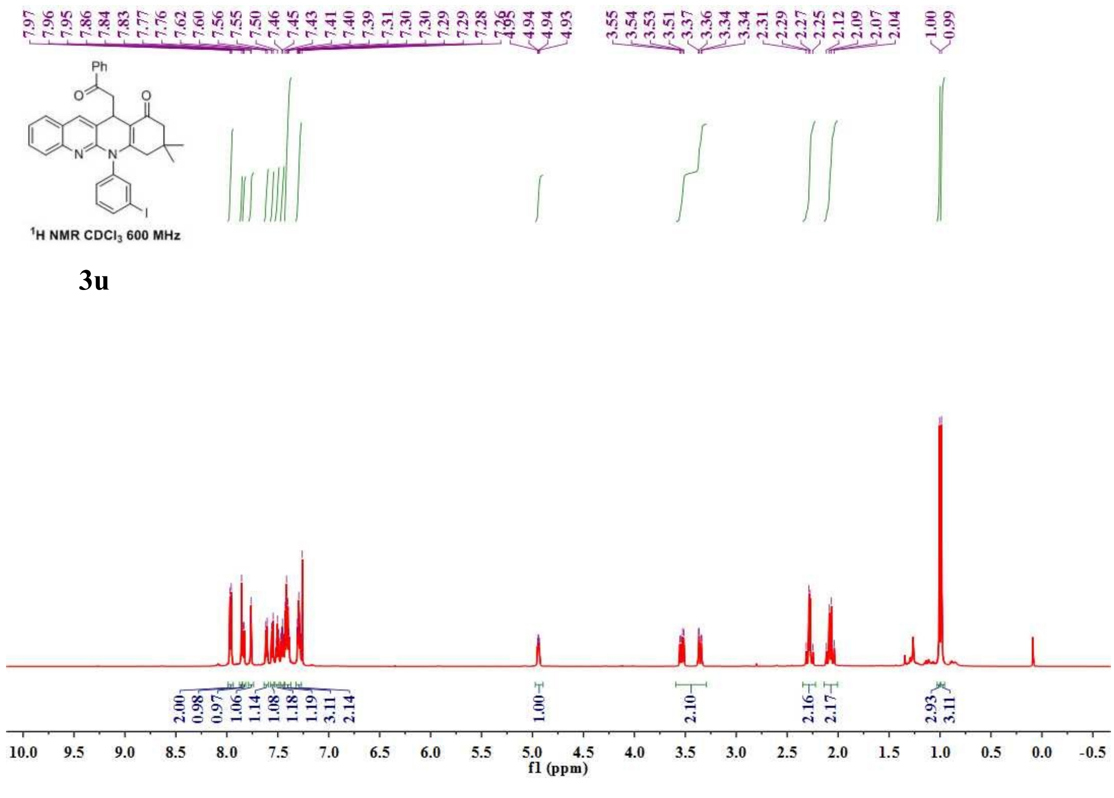
77.2
77.0
76.8
50.1
46.6
42.4
32.6
31.6
29.1
27.4
Ph
O
O
N
N
Br
^{13}C NMR CDCl$_3$ 150 MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3t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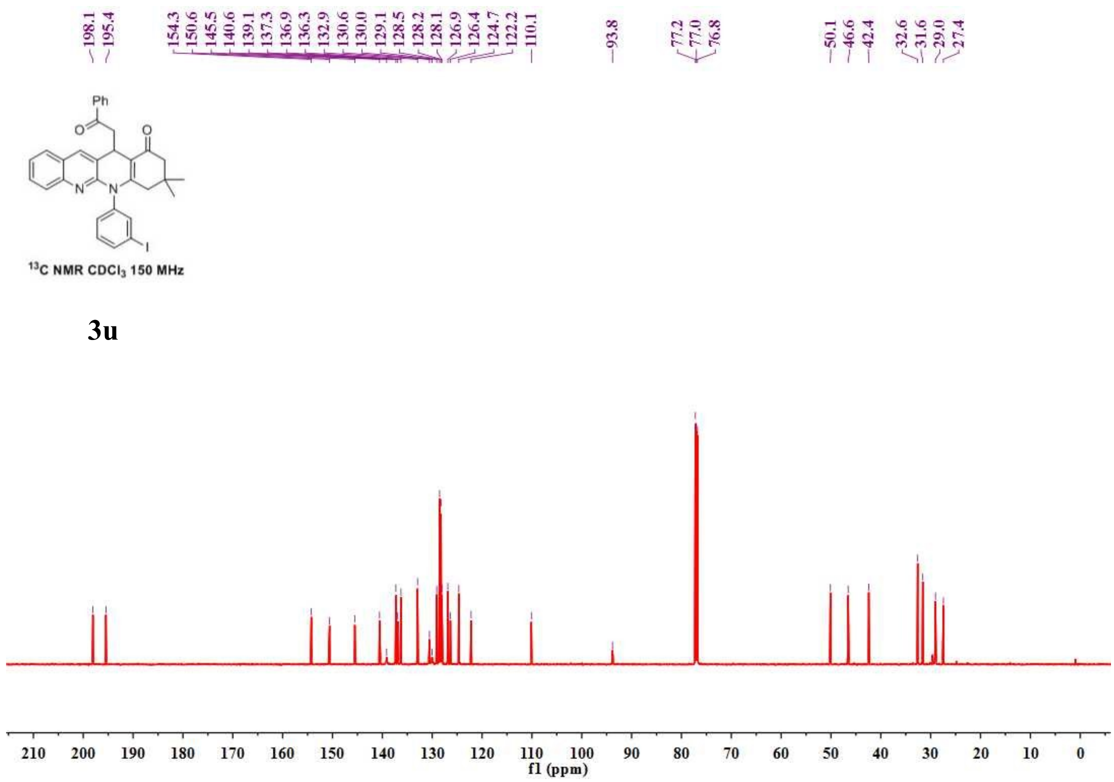
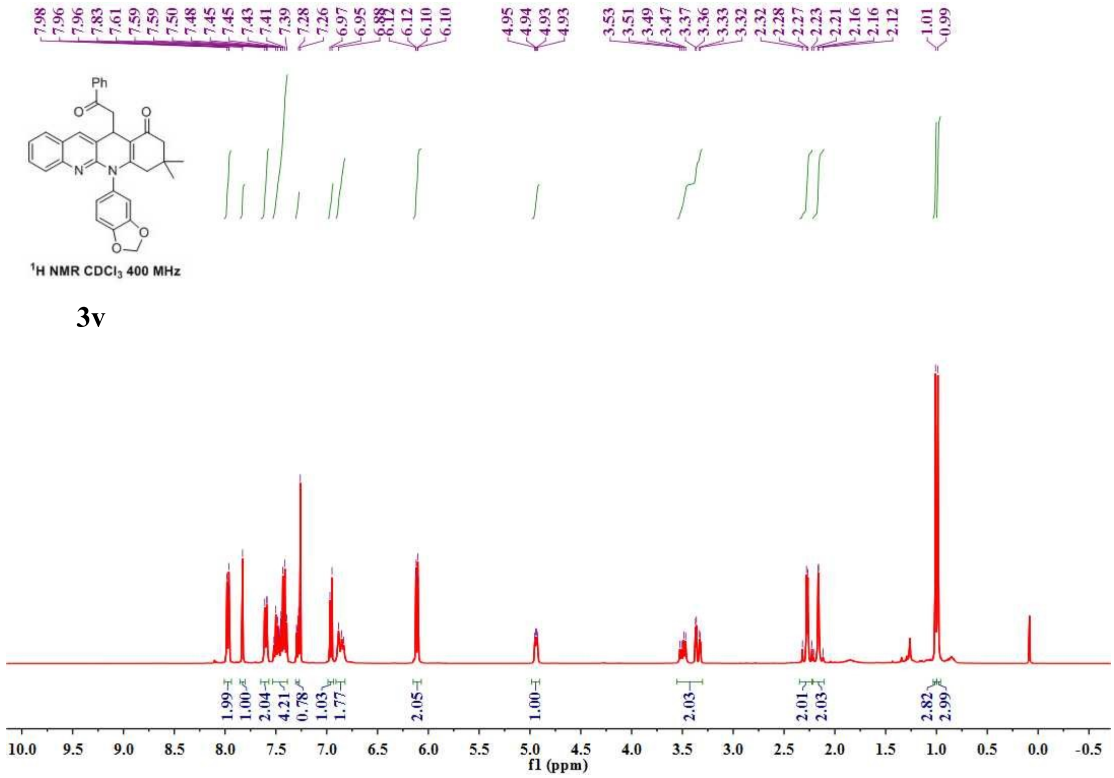
7.50
7.46
7.45
7.43
7.41
7.40
7.39
7.31
7.30
7.30
7.29
7.29
7.28
7.26
4.95
4.94
4.94
4.93
3.55
3.54
3.53
3.51
3.37
3.36
3.34
3.34
2.31
2.29
2.27
2.25
2.12
2.09
2.07
2.04
1.00
0.99
Ph
O
O
N
N
I
^{1}H NMR CDCl$_3$ 600 MHz
2.00
0.98
0.97
1.06
1.14
1.08
1.18
1.19
3.11
2.14
1.00
2.10
2.16
2.17
2.93
3.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

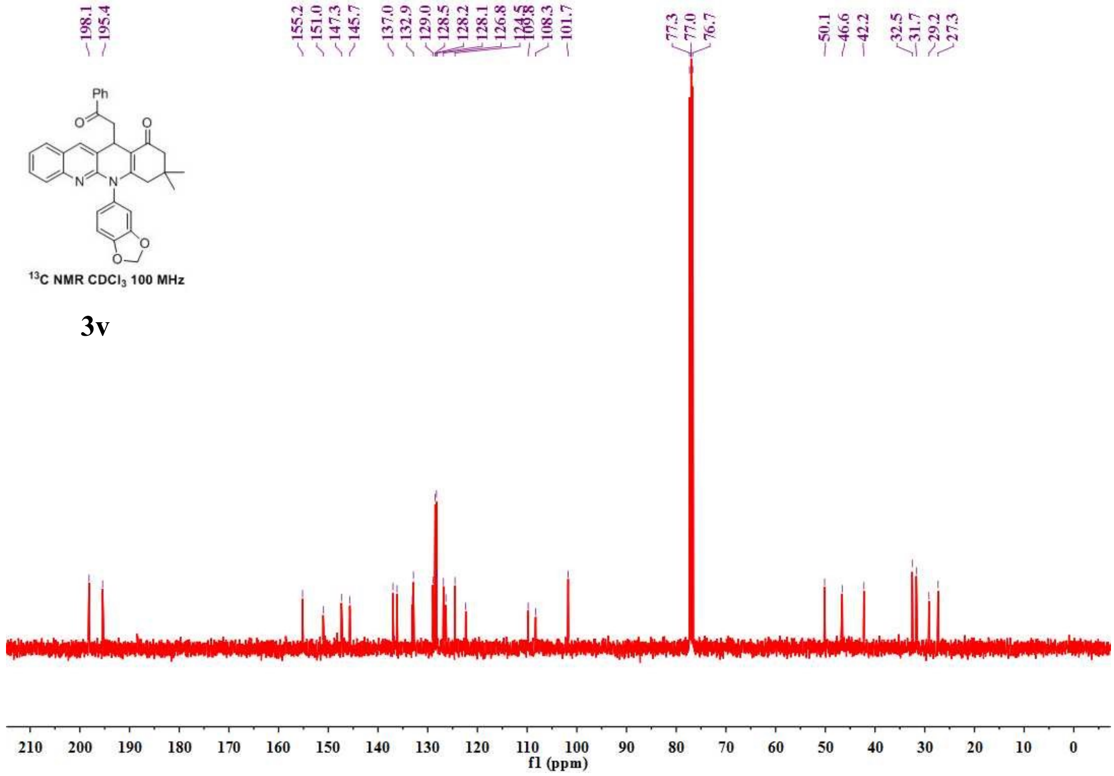
3u



3u



3v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155.2
151.0
147.3
145.7
137.0
132.9
129.0
128.5
128.2
128.1
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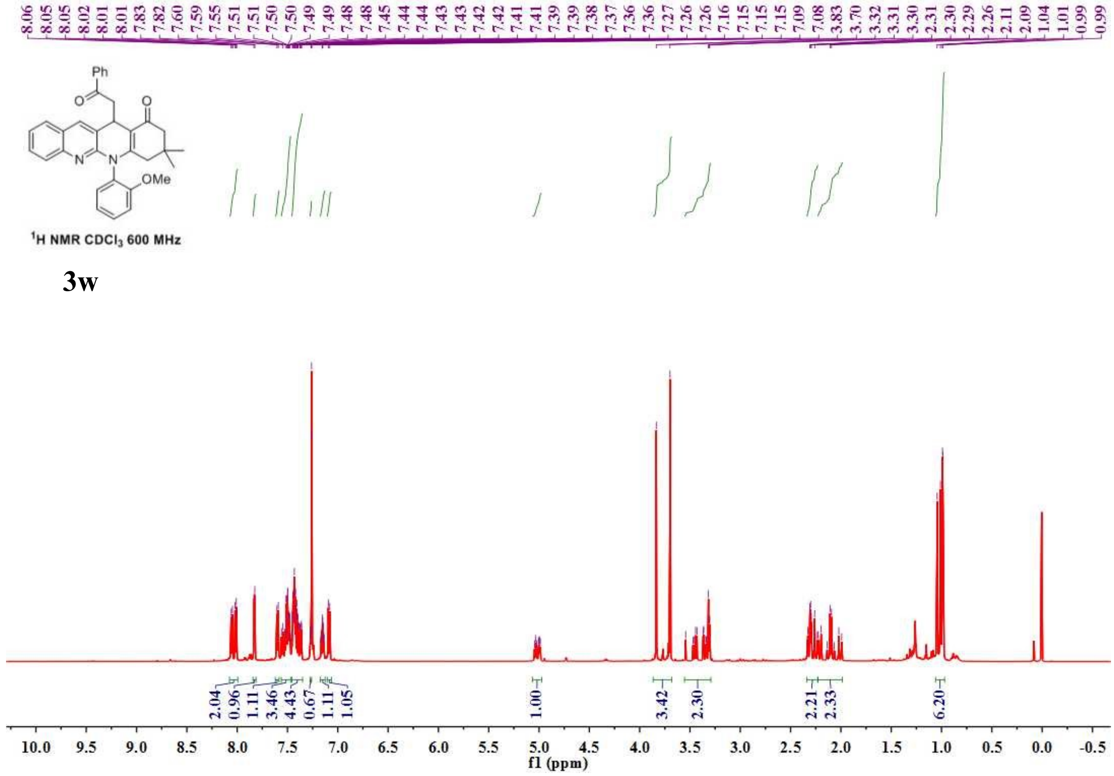
124.5
109.8
108.3
101.7
77.3
77.0
76.7
50.1
46.6
42.2
32.5
31.7
29.2
27.3
Ph
O
O
N
N
O
O
^{13}C NMR CDCl$_3$ 100 MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3v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8.05
8.05
8.02
8.01
8.01
7.83
7.82
7.60
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7.55
7.51
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7.50
7.50
7.49
7.49
7.48
7.48
7.45
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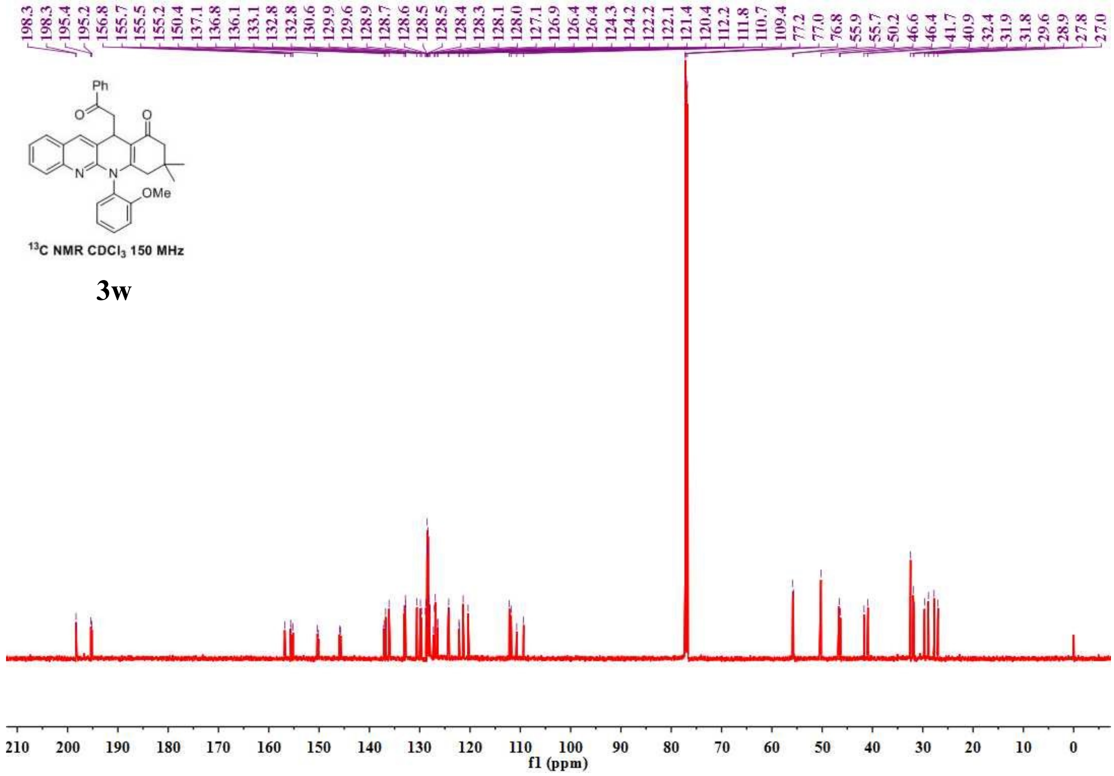
7.43
7.43
7.42
7.42
7.41
7.41
7.39
7.39
7.38
7.37
7.36
7.36
7.27
7.26
7.26
7.16
7.15
7.15
7.15
7.09
7.08
3.83
3.70
3.32
3.31
3.30
2.31
2.30
2.29
2.26
2.11
2.09
1.04
1.01
0.99
0.99
Ph
O
O
N
N
OMe
^{1}H NMR CDCl$_3$ 600 MHz
2.04
0.96
1.11
3.46
4.43
0.67
1.11
1.05
1.00
3.42
2.30
2.21
2.33
6.20
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3w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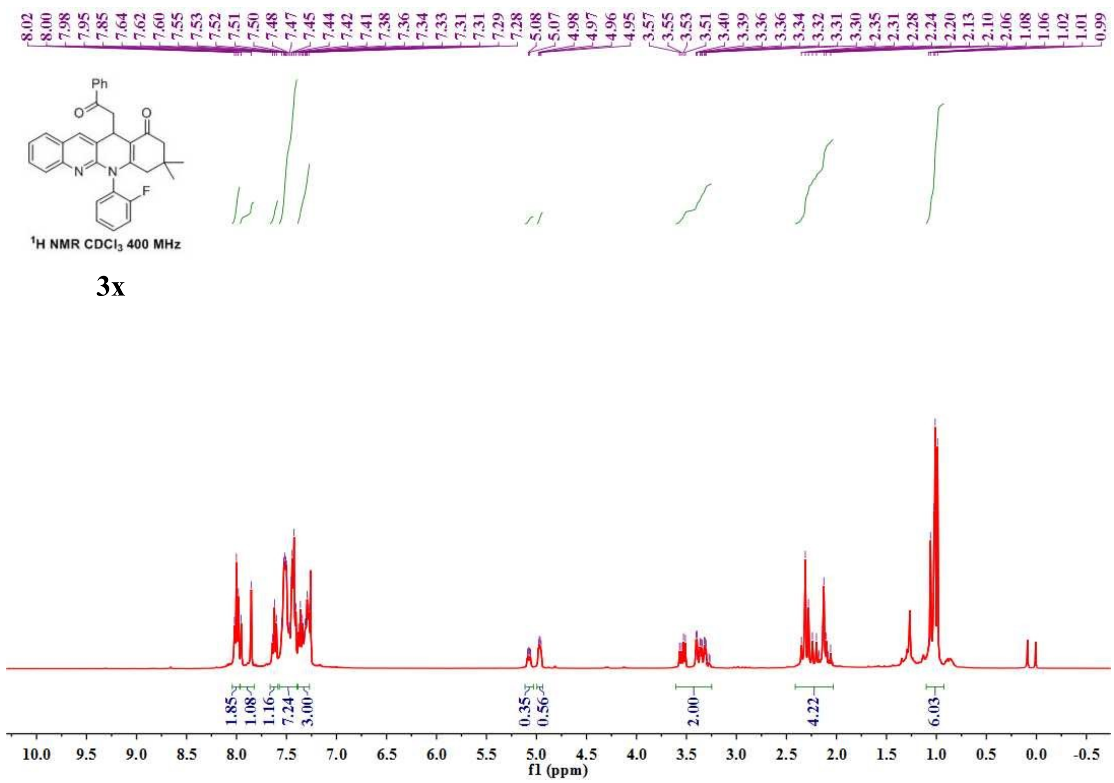
Ph
O
O
N
N
OMe
^{13}C NMR CDCl$_3$ 150 MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3w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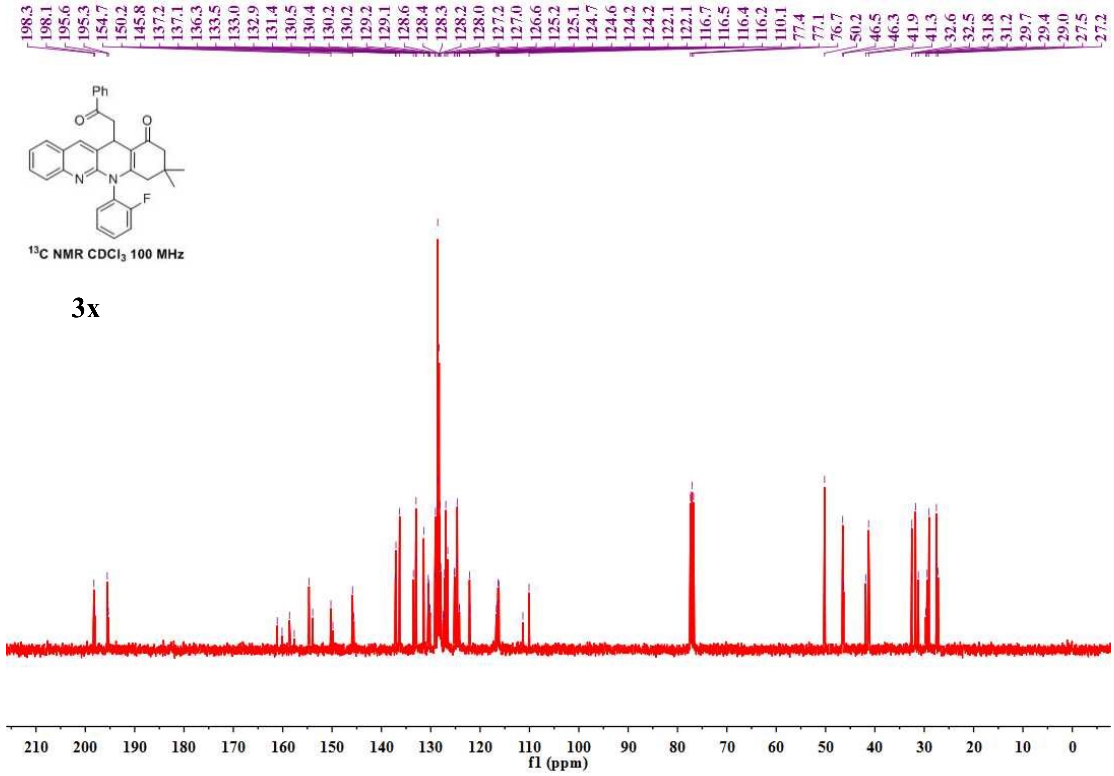
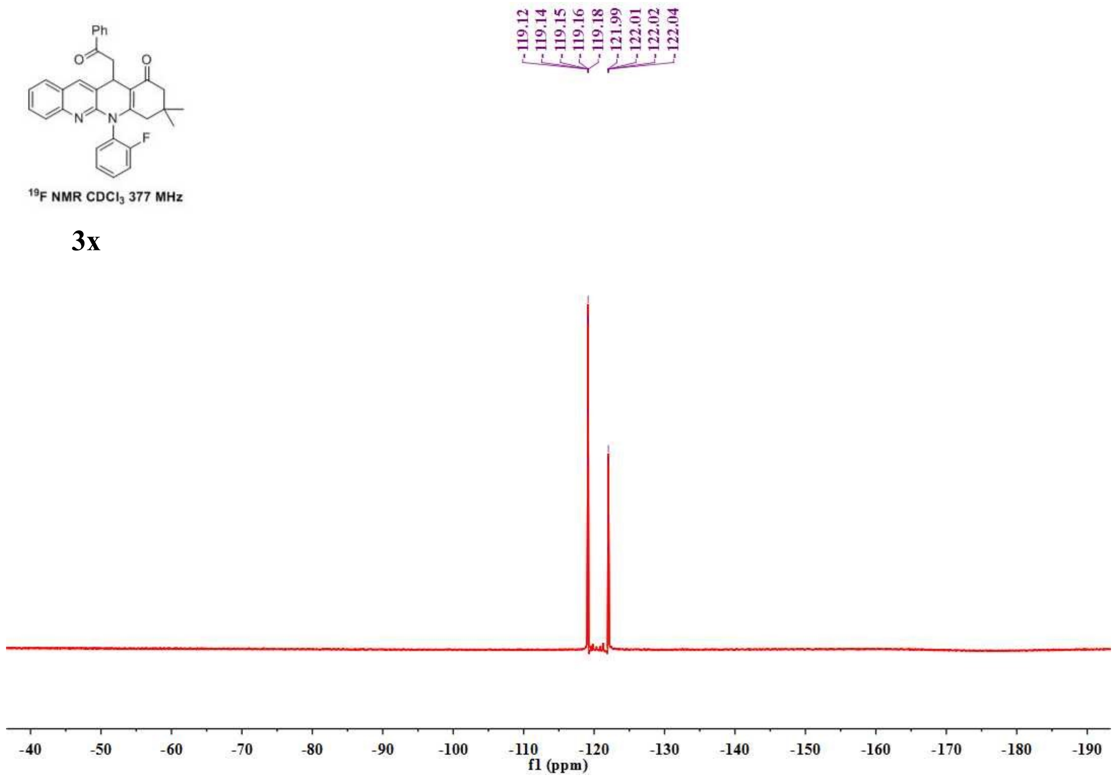
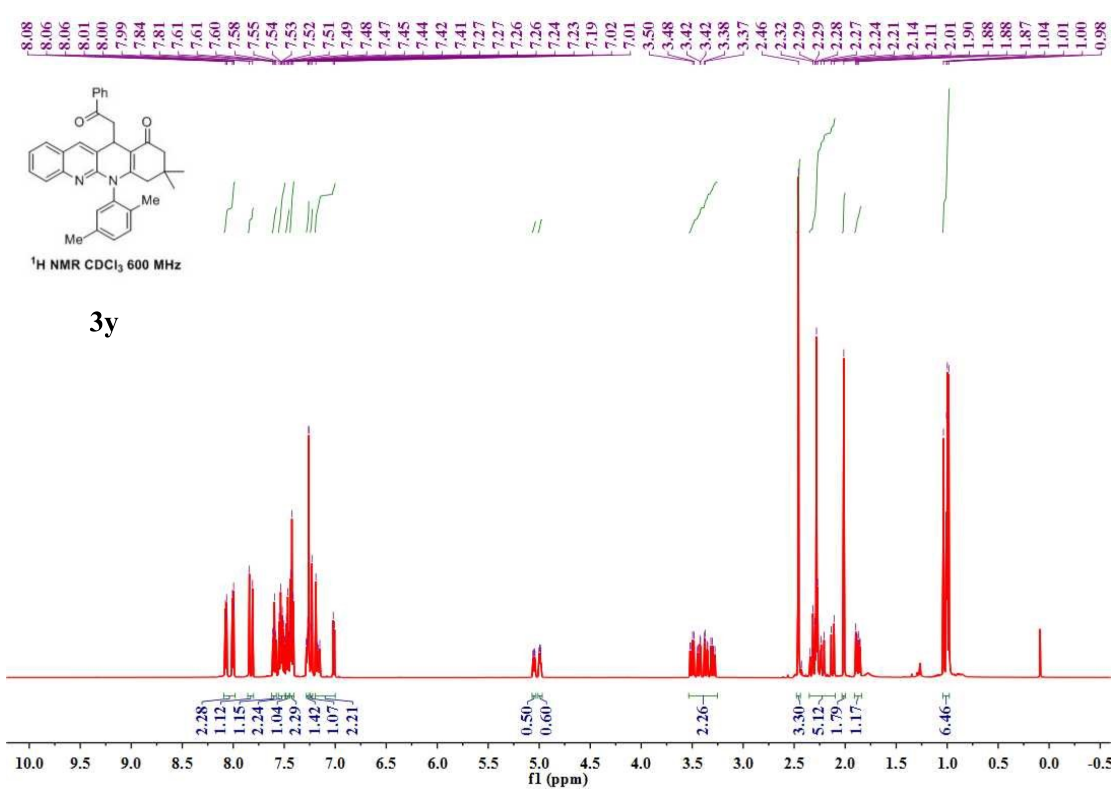
Ph
O
O
N
N
F
^{1}H NMR CDCl$_3$ 400 MHz
1.85 1.08 1.16 7.24 3.00 0.35 0.56 2.00 4.22 6.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

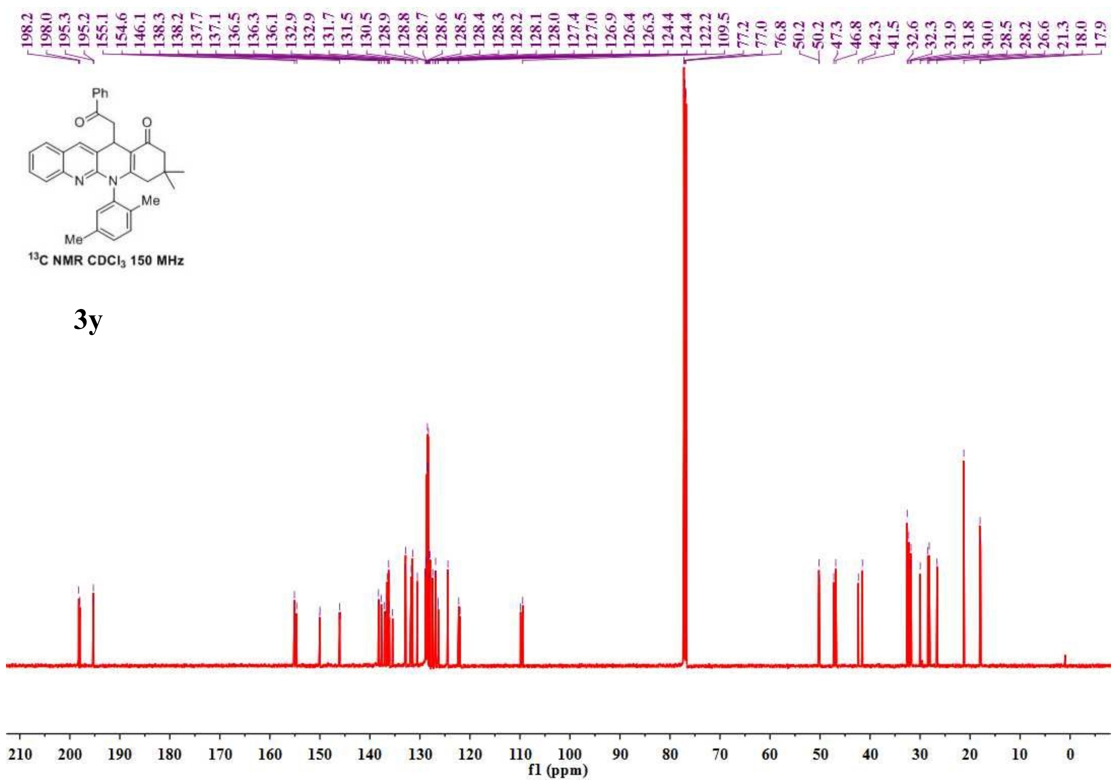
3x


198.3 198.1 195.6 195.3 154.7 150.2 145.8 137.2 137.1 136.3 133.5 133.0 132.9 131.4 130.5 130.4 130.2 130.2 129.2 129.1 128.6 128.4 128.3 128.2 128.0 127.2 127.0 126.6 125.2 125.1 124.7 124.6 124.2 124.2 122.1 122.1 116.7 116.5 116.4 116.2 110.1 77.4 77.1 76.7 50.2 46.5 46.3 41.9 41.3 32.6 32.5 31.8 31.2 29.7 29.4 29.0 27.5 27.2
Ph
O
O
N
N
F
13C NMR CDCl3 100 MHz
3x
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

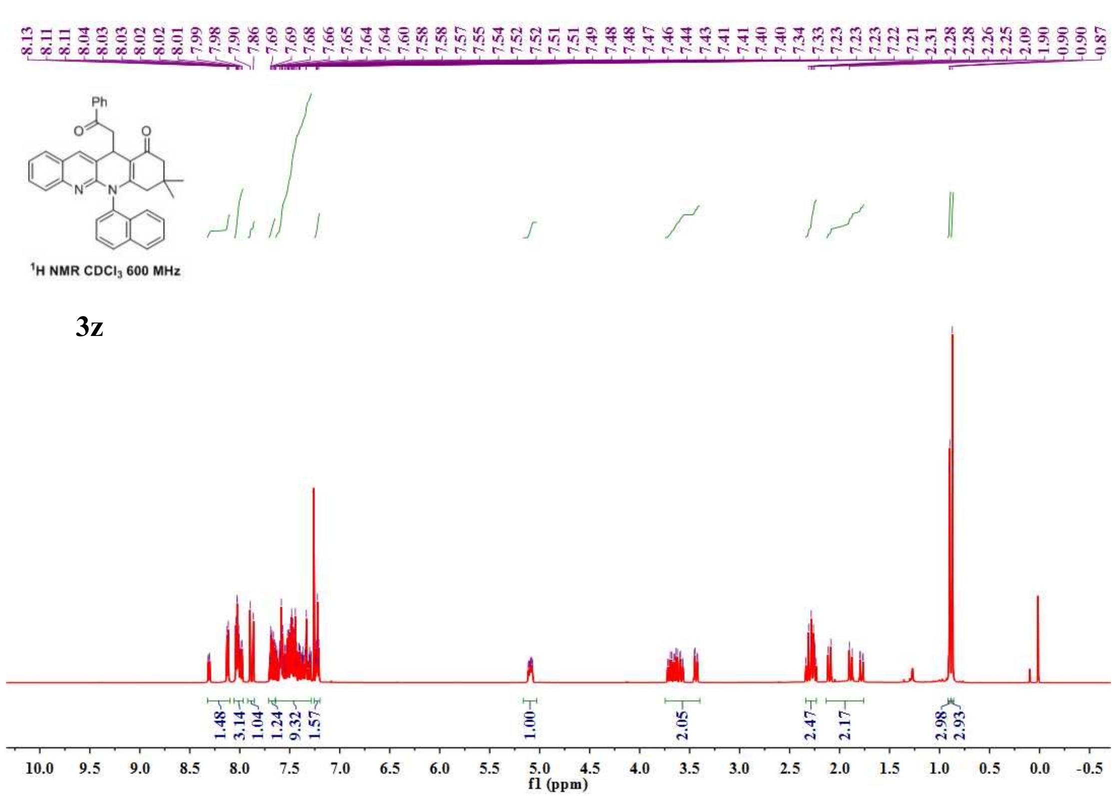

119.12 119.14 119.15 119.16 119.18 121.99 122.01 122.02 122.04
Ph
O
O
N
N
F
19F NMR CDCl3 377 MHz
3x
-40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)



3y



3y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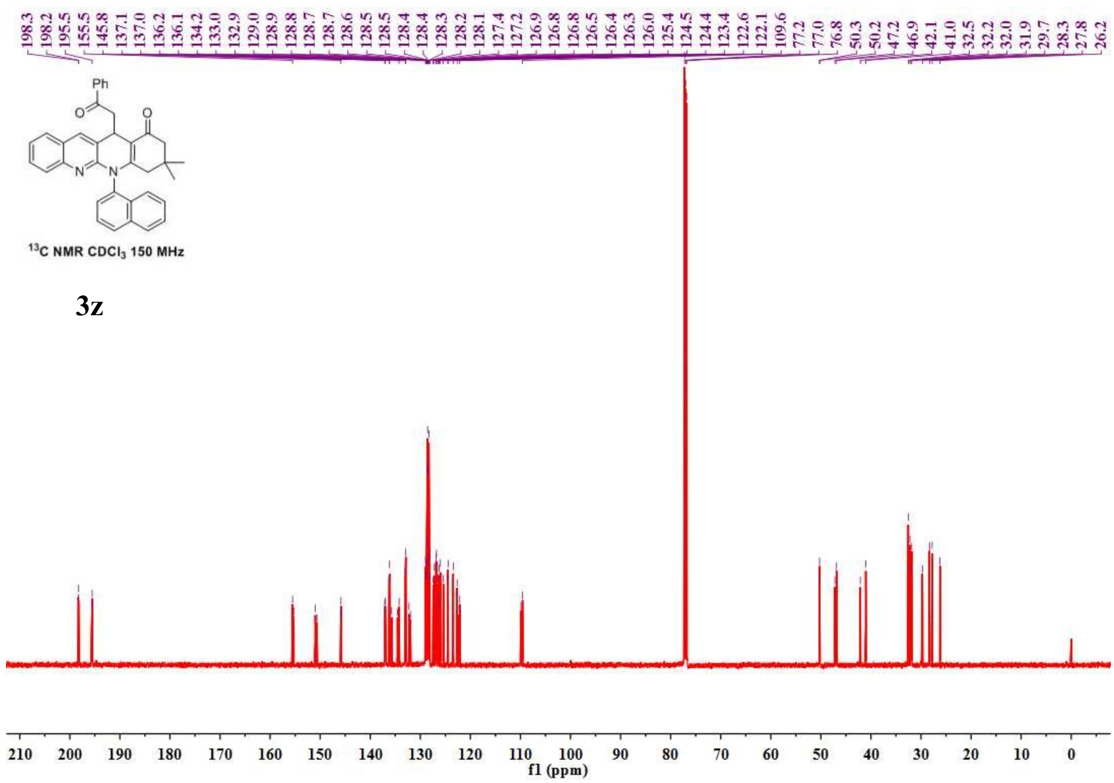
Ph
O
O
N
N
^{1}H NMR CDCl$_3$ 600 MHz
3z
1.48 3.14 1.04 1.24 9.32 1.57 1.00 2.05 2.47 2.17 2.98 2.93
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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Ph
O
O
N
N
^{13}C NMR CDCl$_3$ 150 MHz
3z
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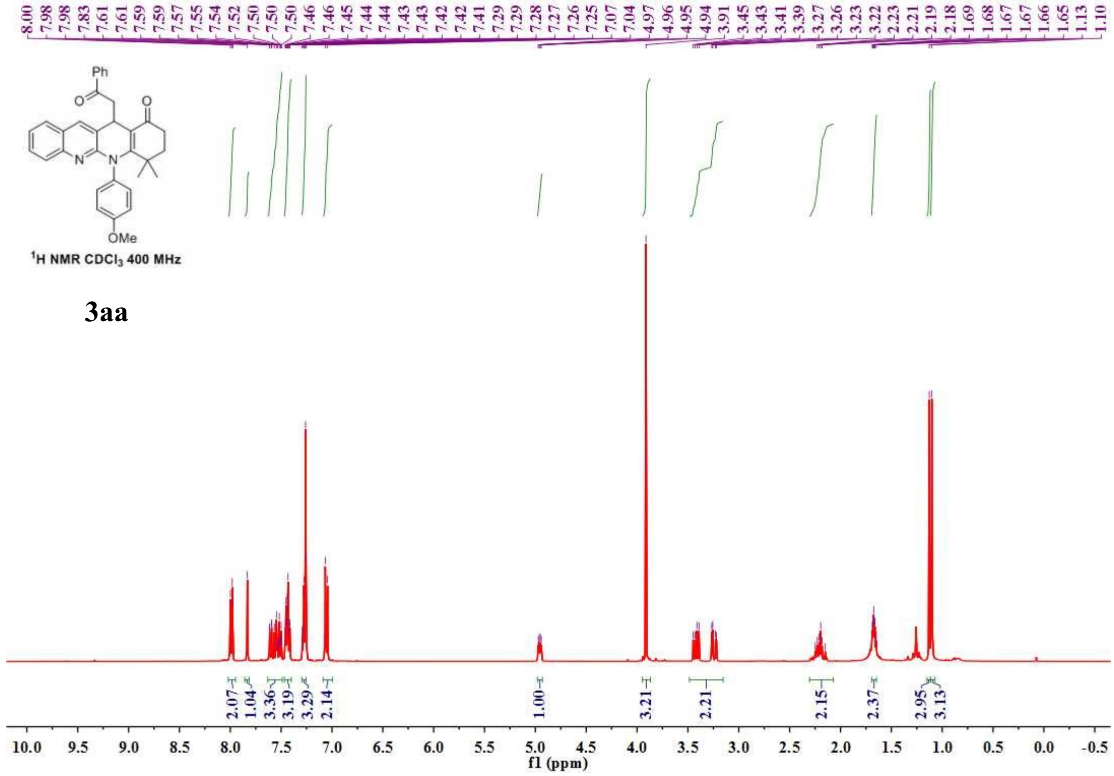
f1 (ppm)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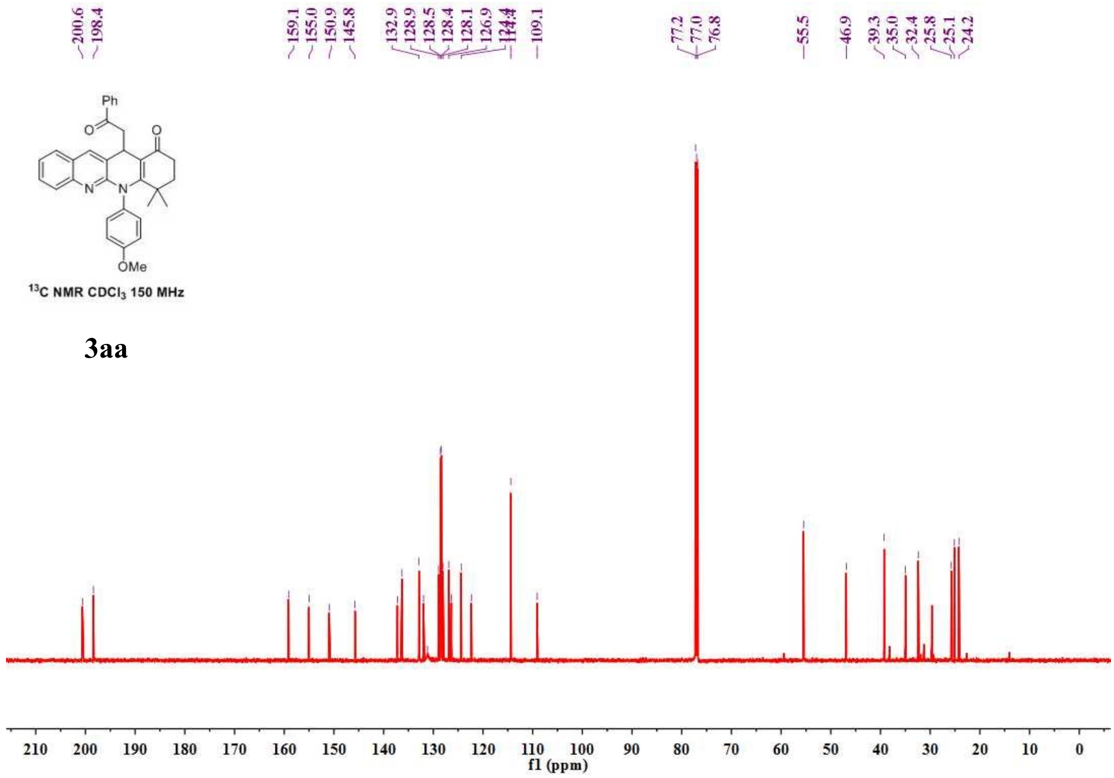
Ph
O
N
N
OMe
1H NMR CDCl3 400 MHz
3aa
2.07 1.04 3.36 3.19 3.29 2.14 1.00 3.21 2.21 2.15 2.37 2.95 3.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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Ph
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OMe
13C NMR CDCl3 150 MHz
3aa
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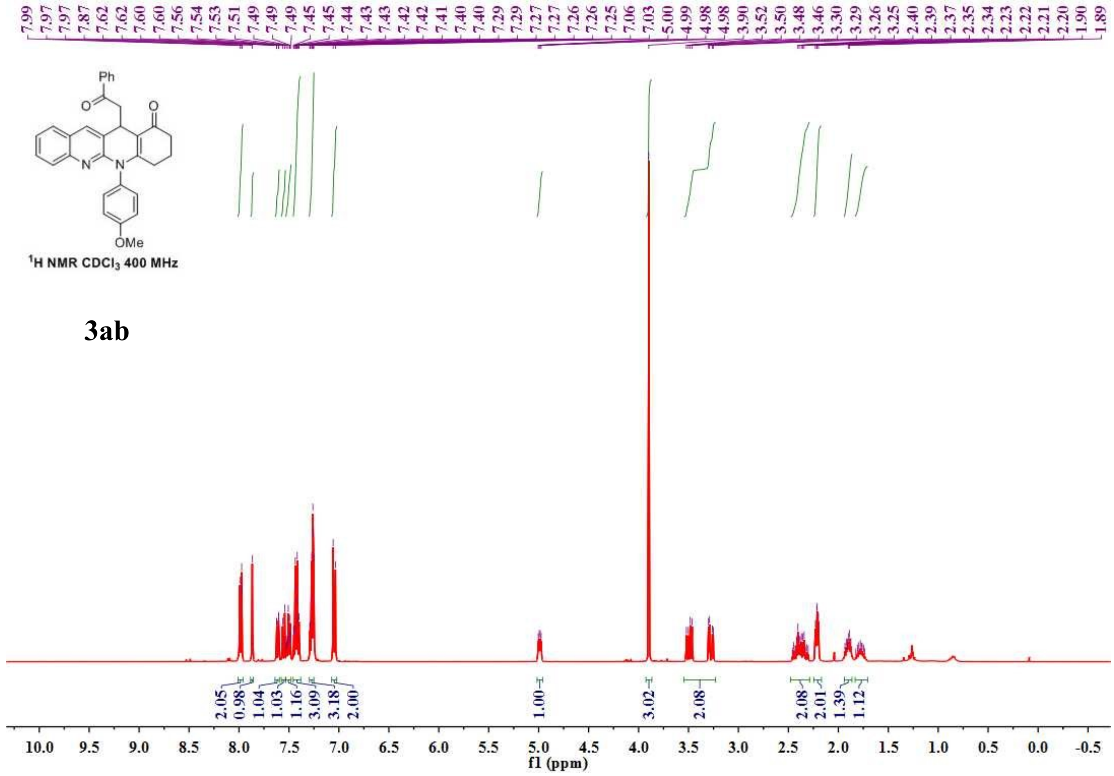
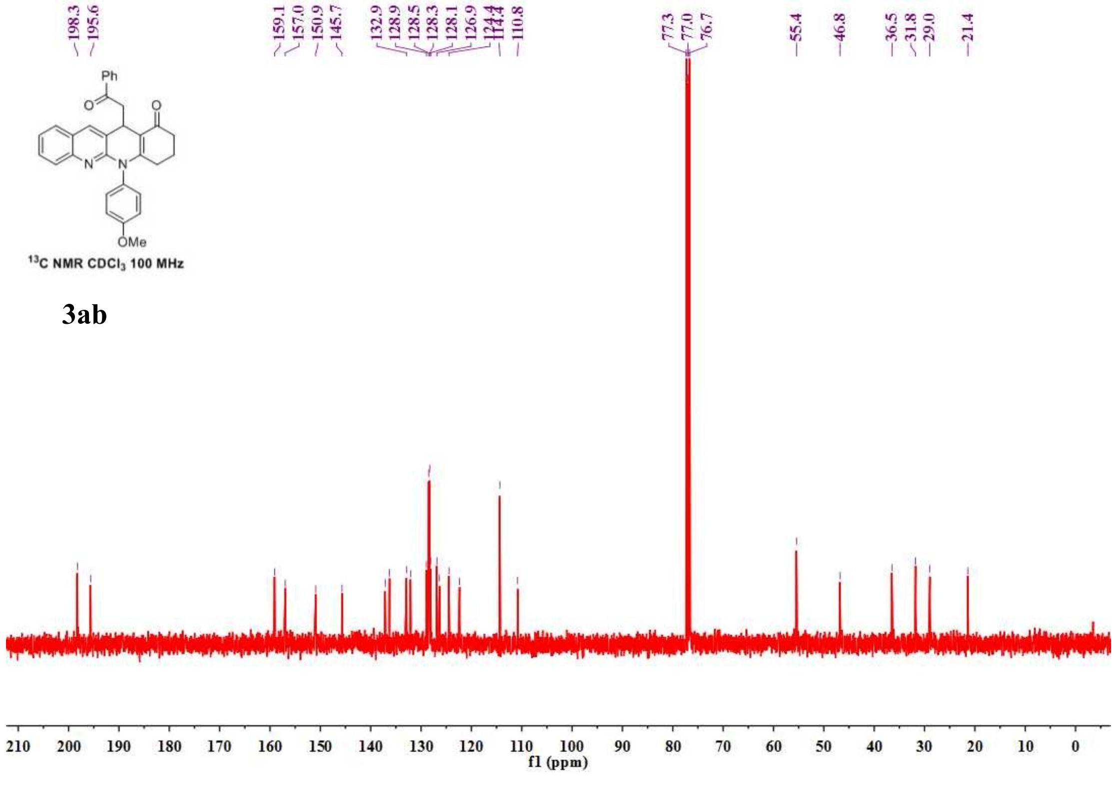
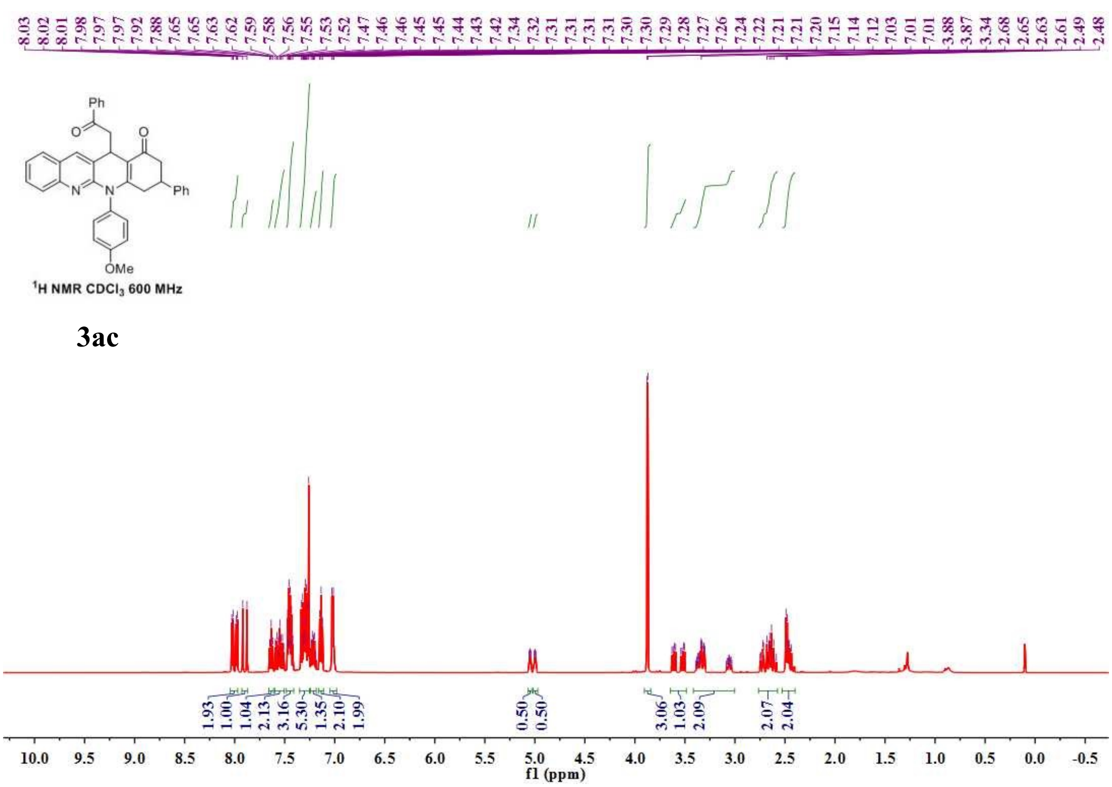
f1 (ppm)



3ab



3ab



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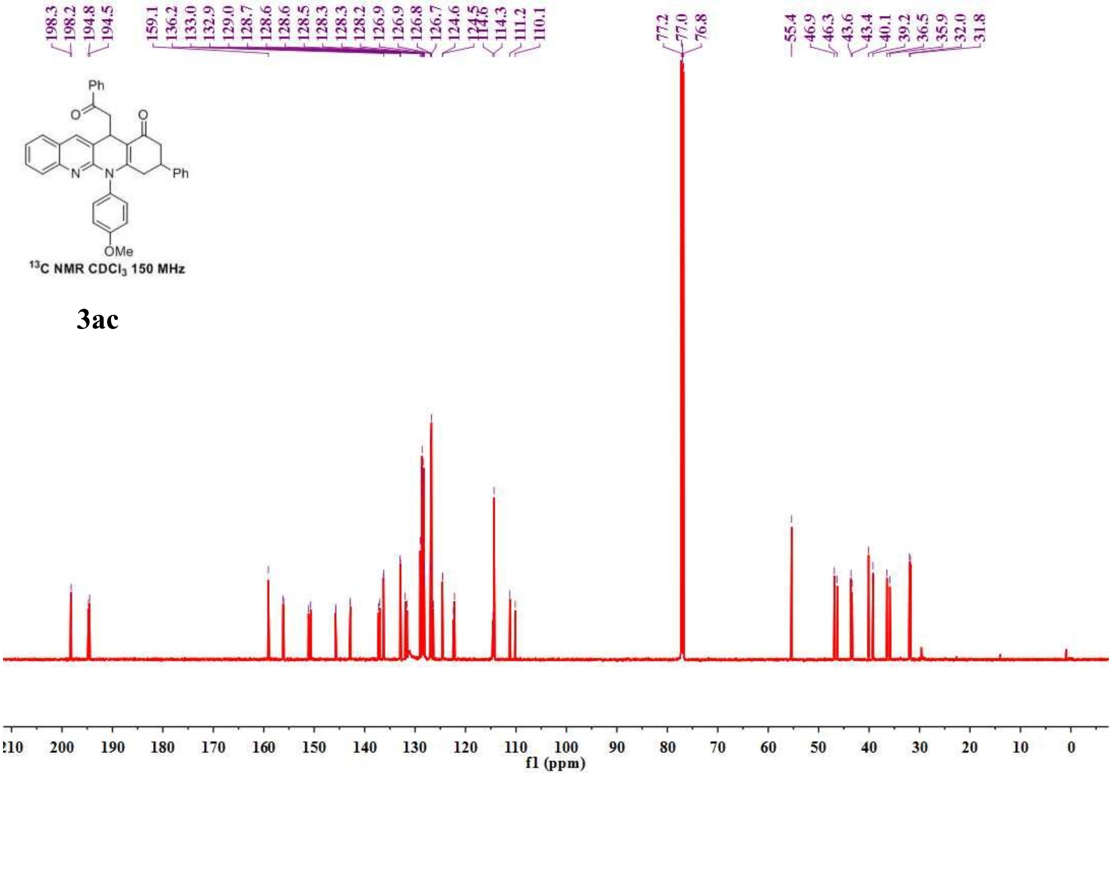

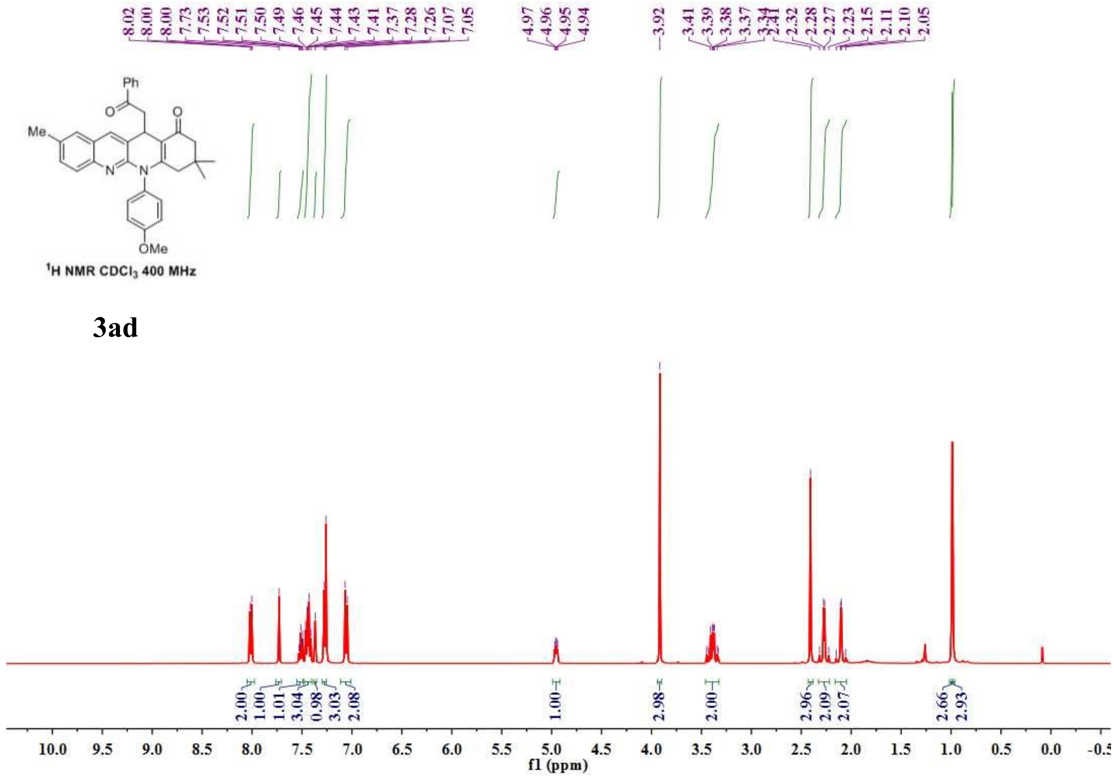
Ph
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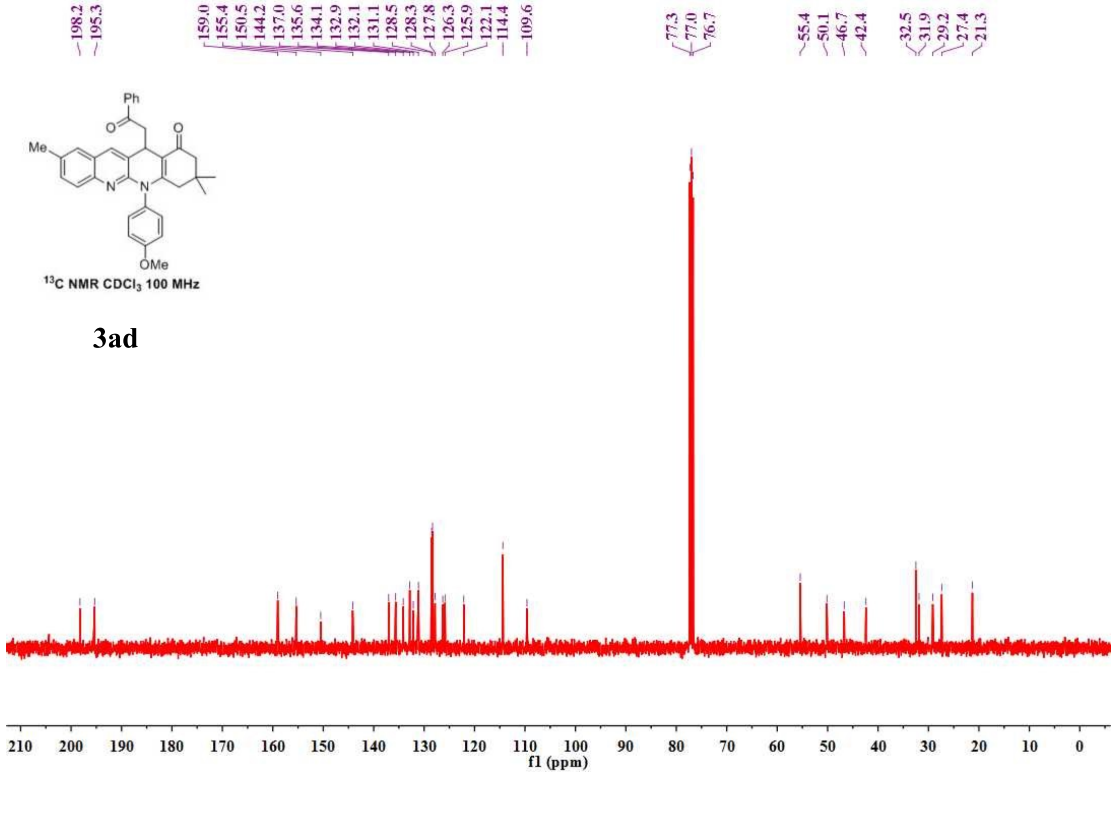
Me
N
N
O
OMe
¹H NMR CDCl3 400 MHz
f1 (ppm)

3ad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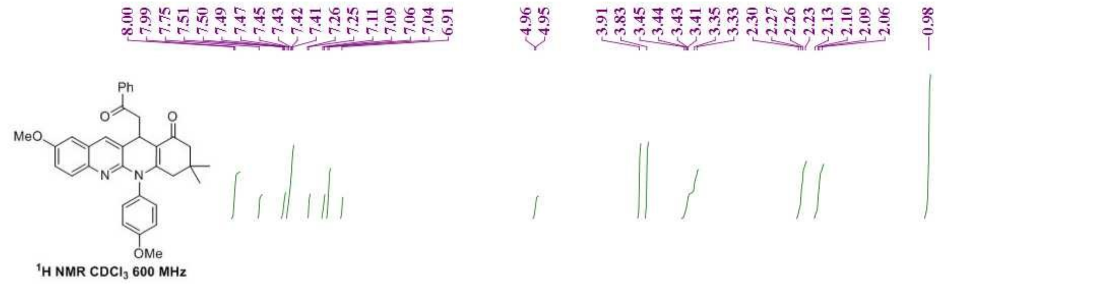
Me
N
N
O
OMe
¹³C NMR CDCl3 100 MHz
f1 (ppm)

3ad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7.43
7.42
7.41
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7.11
7.09
7.06
7.04
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4.95
3.91
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3.41
3.35
3.33
2.30
2.27
2.26
2.23
2.13
2.10
2.09
2.06
0.98
Ph
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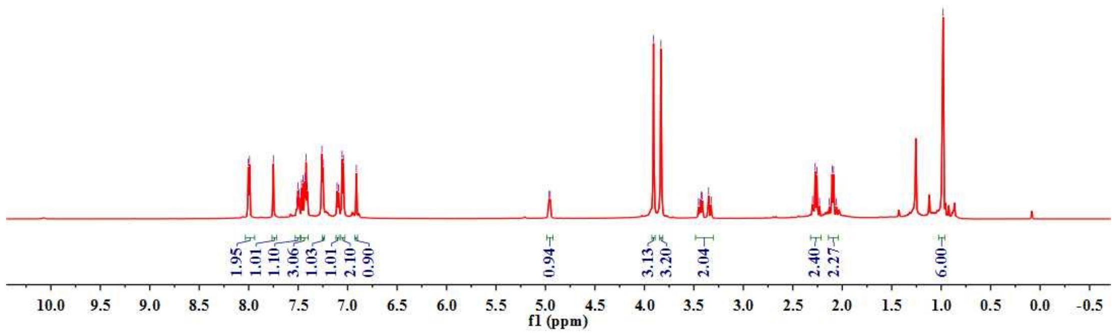
MeO
N
N
OMe
^{1}H NMR CDCl$_3$ 600 MHz

3ae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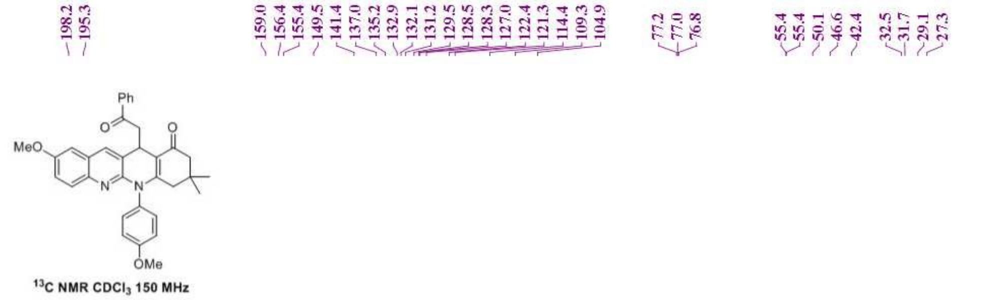
1.10
3.06
1.03
1.01
2.10
0.90
0.94
3.13
3.20
2.04
2.40
2.27
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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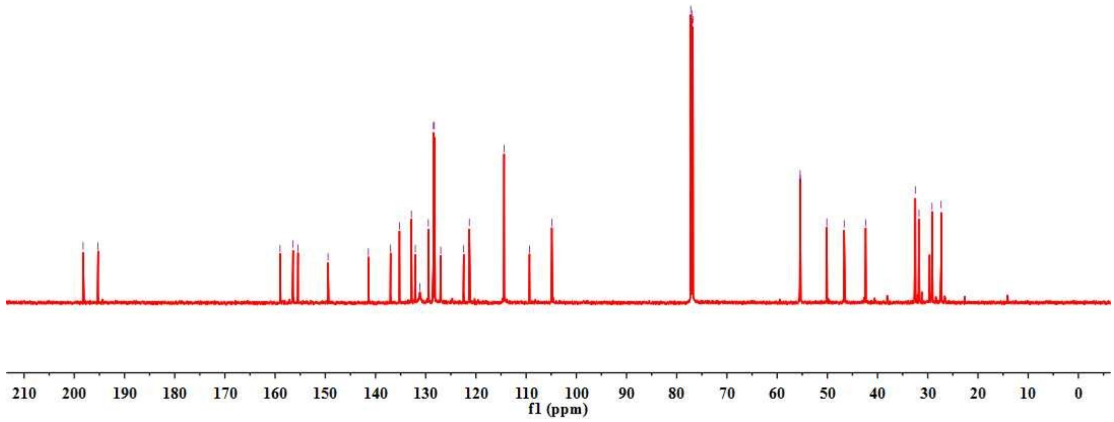
156.4
155.4
149.5
141.4
137.0
135.2
132.9
132.1
131.2
129.5
128.5
128.3
127.0
122.4
121.3
114.4
109.3
104.9
77.2
77.0
76.8
55.4
55.4
50.1
46.6
42.4
32.5
31.7
29.1
27.3
Ph
O
O
MeO
N
N
OMe
^{13}C NMR CDCl$_3$ 150 MHz

3ae


210
200
190
180
170
160
150
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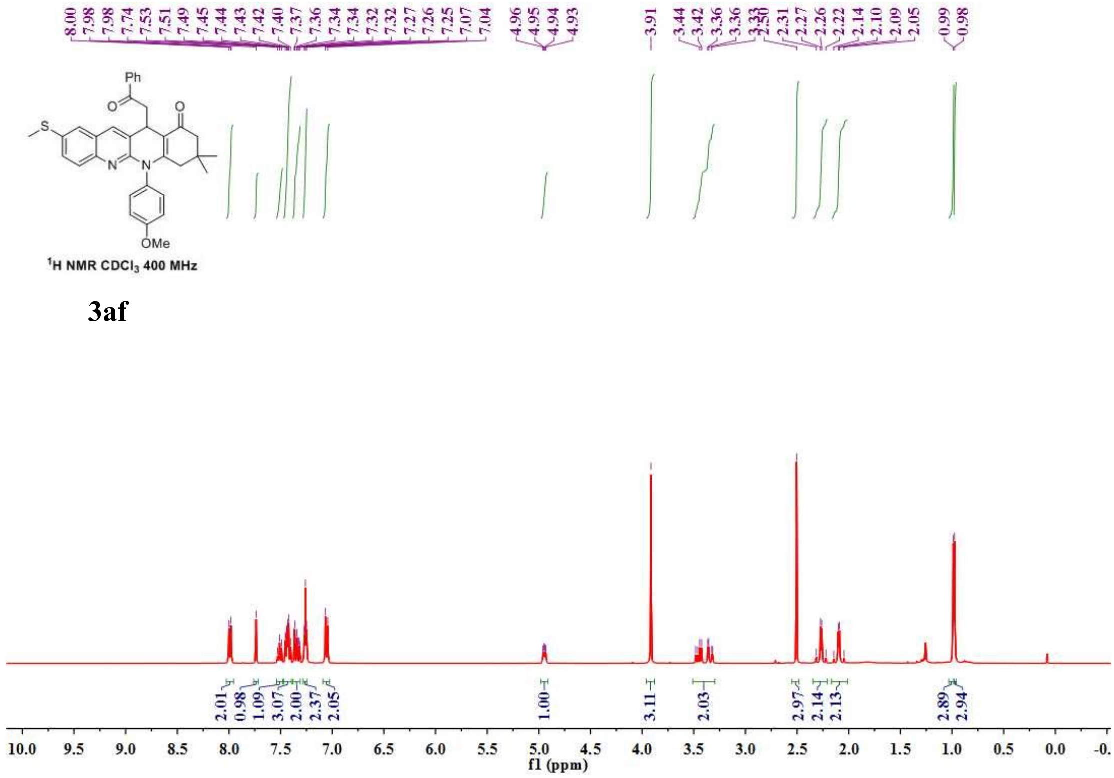
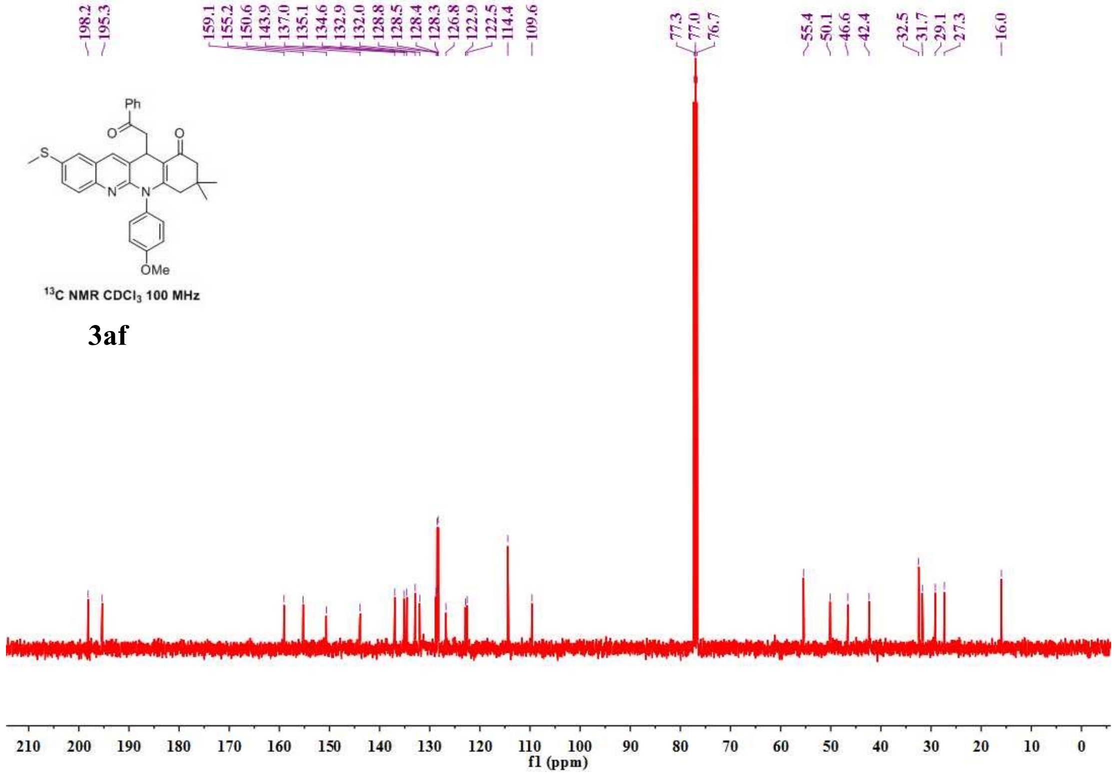
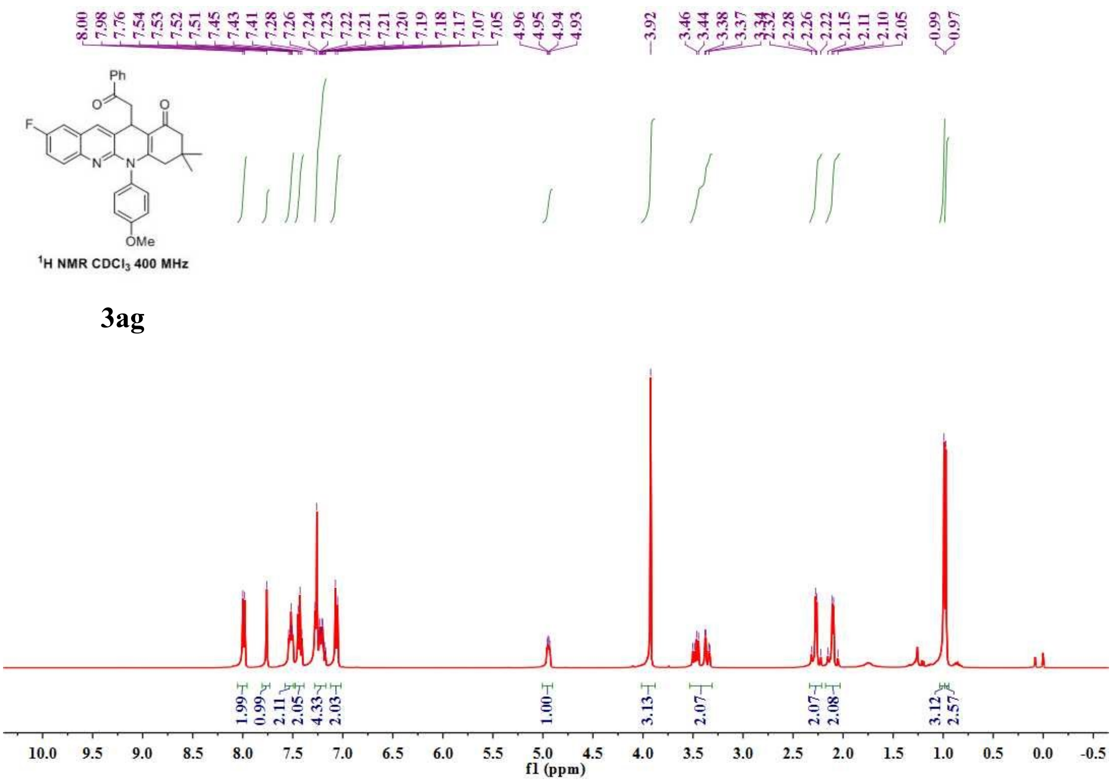
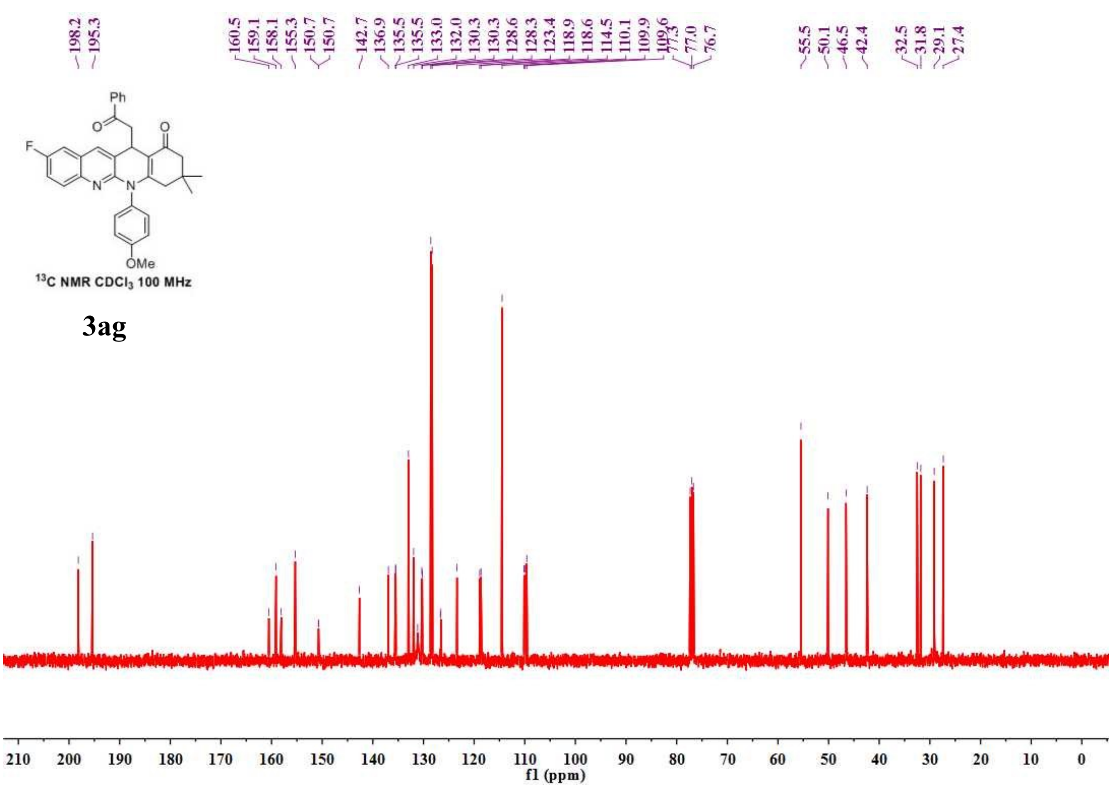
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Ph
O
S
N
N
OMe
1H NMR CDCl3 400 MHz
3af
f1 (ppm)

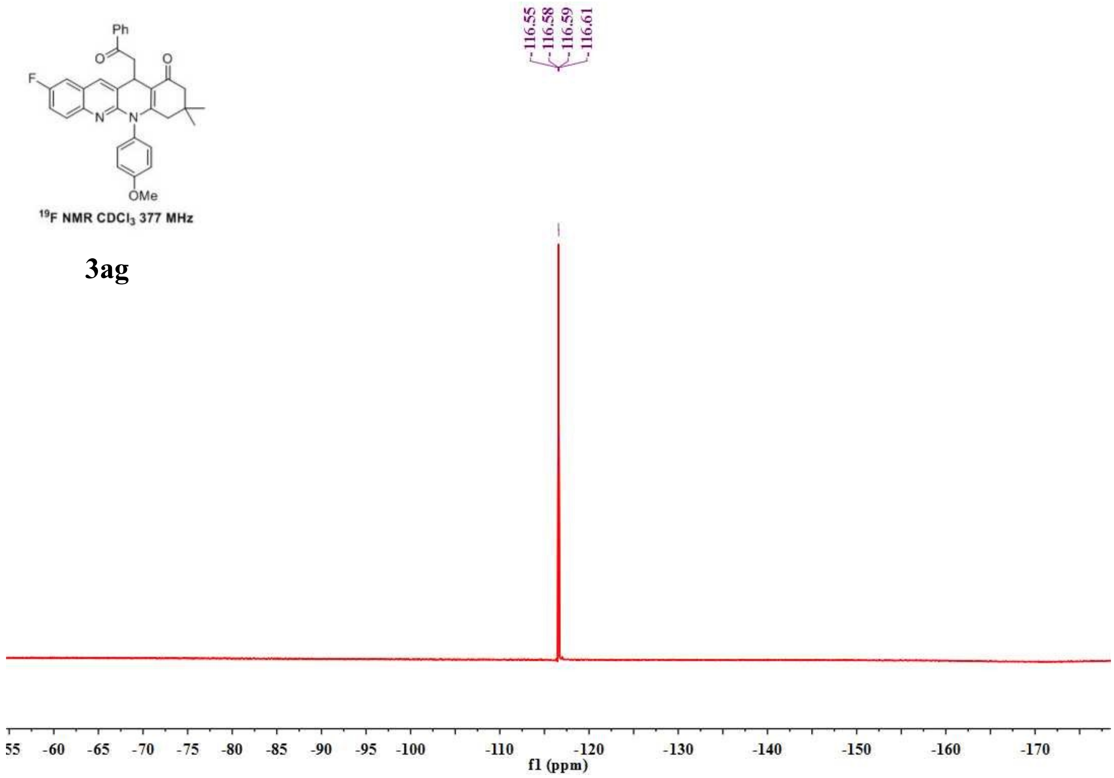

Ph
O
S
N
N
OMe
13C NMR CDCl3 100 MHz
3af
f1 (ppm)



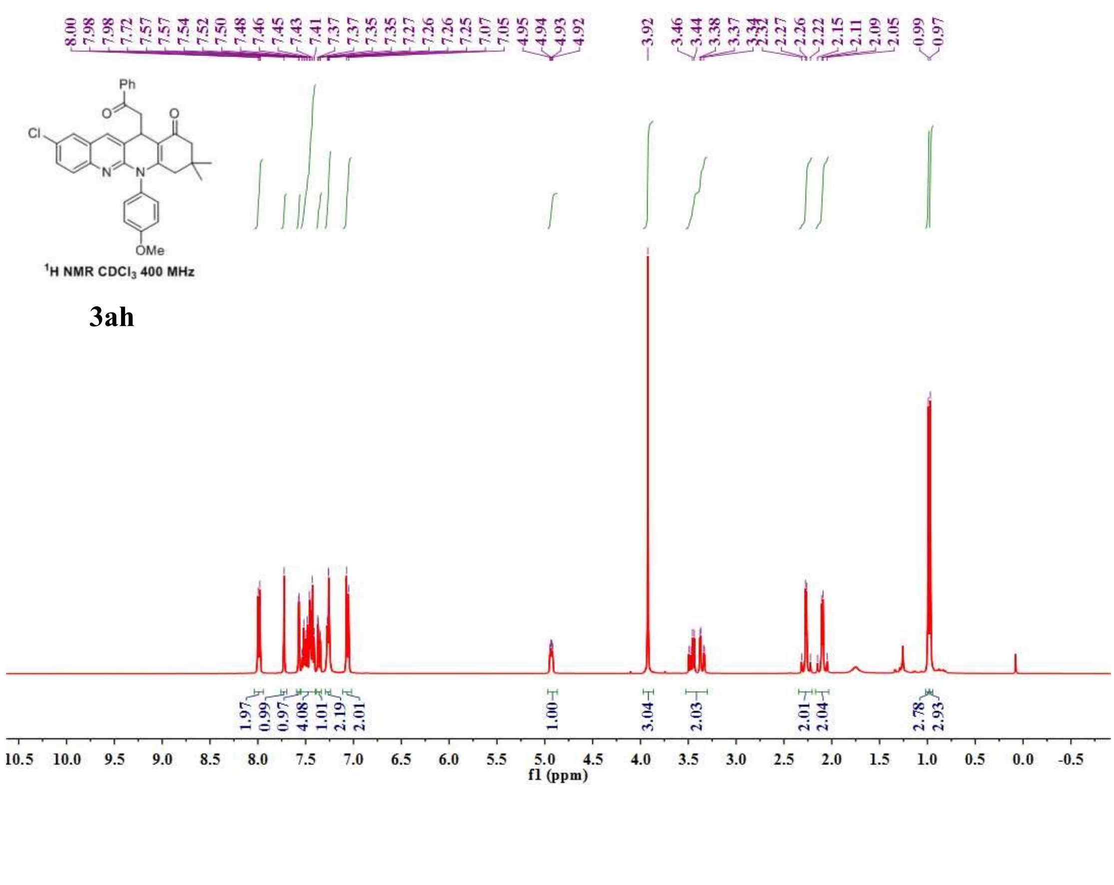
3ag



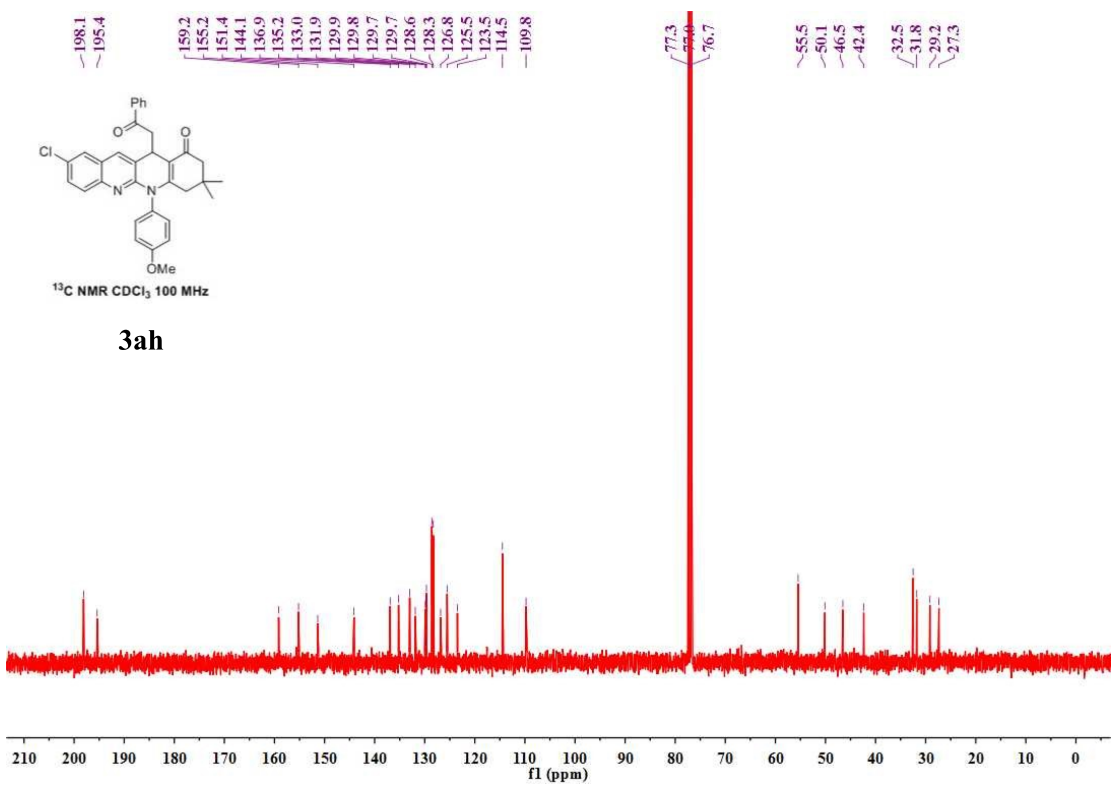
3ag


-116.55
-116.58
-116.59
-116.61
^{19}F NMR CDCl$_3$ 377 MHz
f1 (ppm)

3ag


8.00 7.98 7.72 7.57 7.57 7.54 7.52 7.50 7.48 7.46 7.45 7.43 7.41 7.37 7.35 7.27 7.26 7.25 7.07 7.05 4.95 4.94 4.93 4.92
3.92
3.46 3.44 3.38 3.37 3.34 3.32 2.27 2.26 2.22 2.15 2.11 2.09 2.05 0.99 0.97
^{1}H NMR CDCl$_3$ 400 MHz
1.97 0.99 0.97 4.08 1.01 2.19 2.01 1.00 3.04 2.03 2.01 2.04 2.78 2.93
f1 (ppm)

3ah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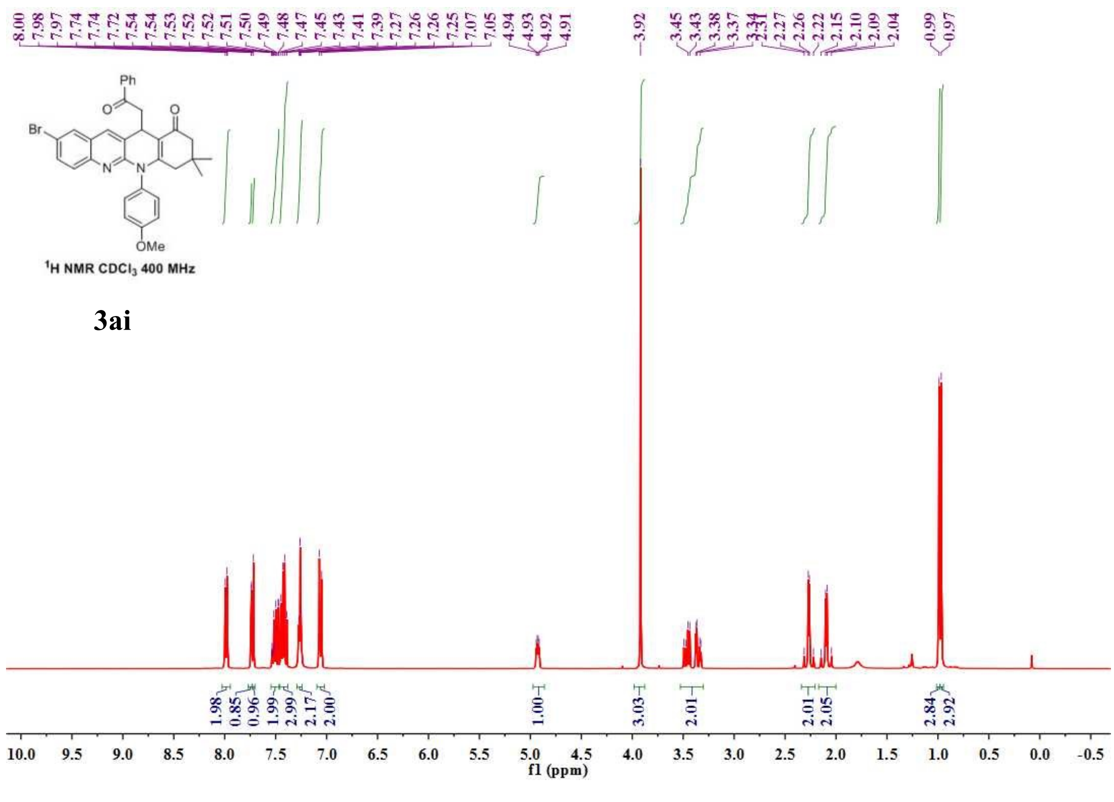
195.4
159.2
155.2
151.4
144.1
136.9
135.2
133.0
131.9
129.9
129.8
129.7
129.7
128.6
128.3
126.8
125.5
123.5
114.5
109.8
77.3
77.0
76.7
55.5
50.1
46.5
42.4
32.5
31.8
29.2
27.3
Ph
O
O
Cl
N
N
OMe
13C NMR CDCl3 100 MHz
f1 (ppm)

3ah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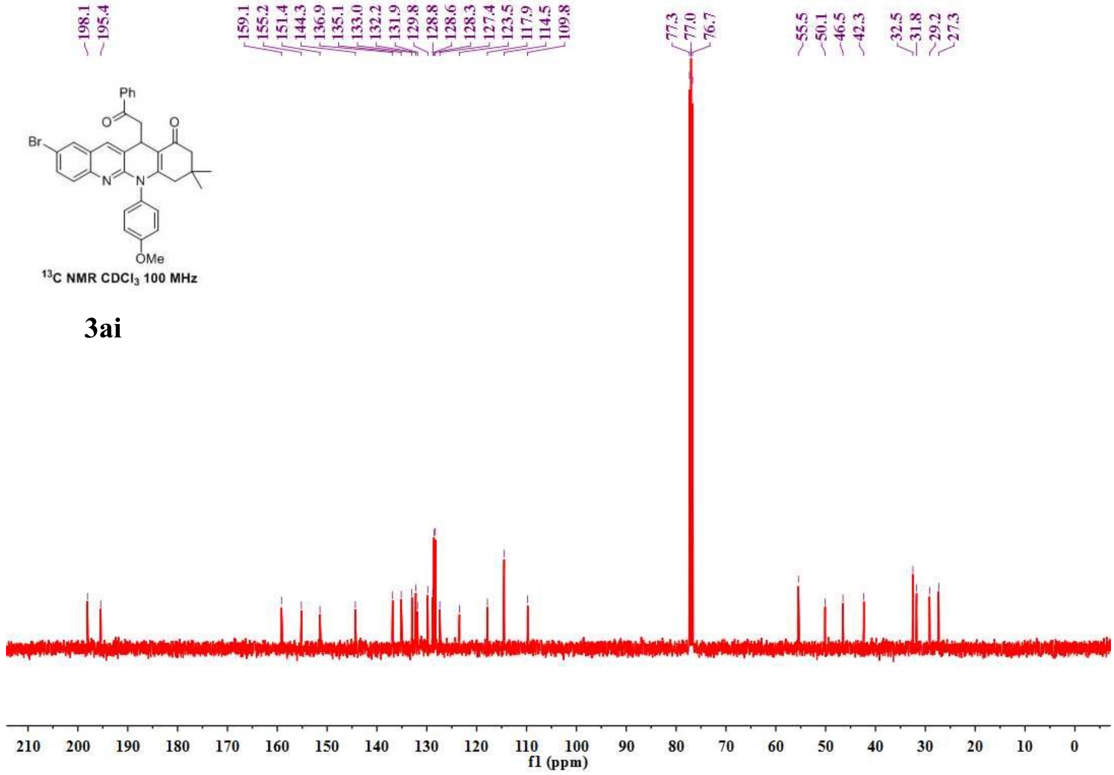
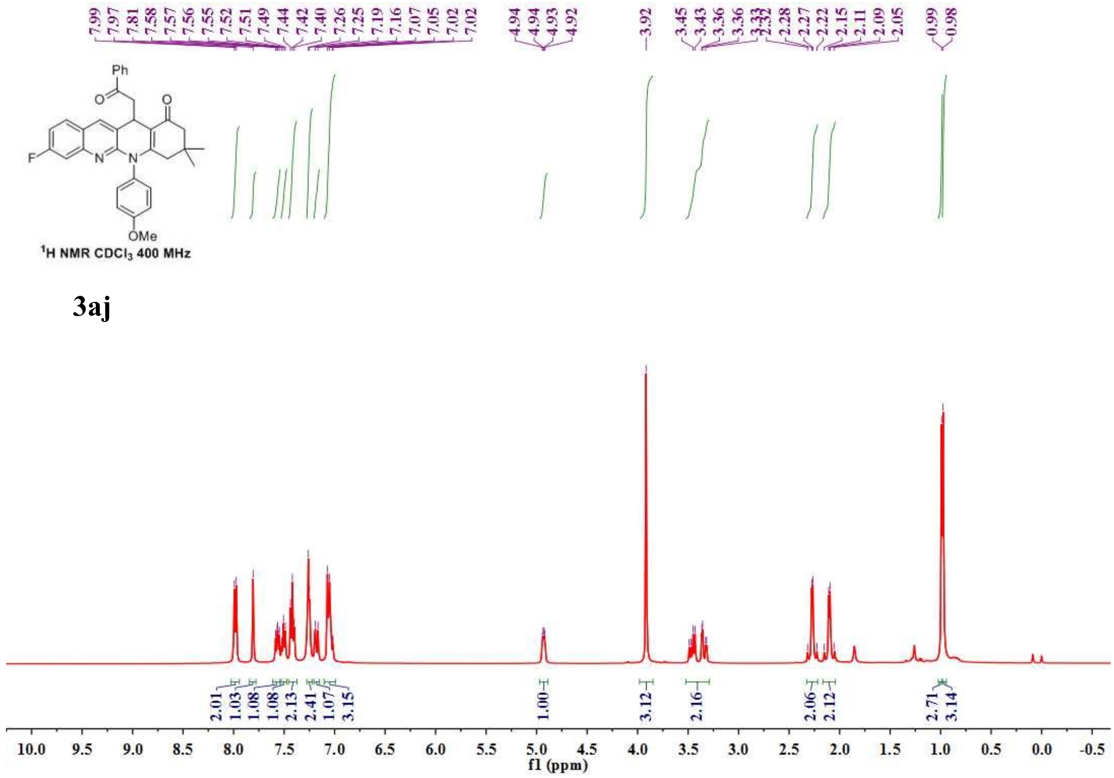
7.98
7.97
7.74
7.74
7.72
7.54
7.54
7.53
7.52
7.52
7.51
7.50
7.49
7.48
7.47
7.45
7.43
7.41
7.39
7.27
7.26
7.26
7.25
7.07
7.05
4.94
4.93
4.92
4.91
3.92
3.45
3.43
3.38
3.37
3.34
3.31
2.27
2.26
2.22
2.15
2.10
2.09
2.04
0.99
0.97
Ph
O
O
Br
N
N
OMe
1H NMR CDCl3 400 MHz
1.98
0.85
0.96
1.99
2.99
2.17
2.00
1.00
3.03
2.01
2.01
2.05
2.84
2.92
f1 (ppm)

3ai


Ph
O
O
Br
N
N
OMe
13C NMR CDCl3 100 MHz
198.1
195.4
159.1
155.2
151.4
144.3
136.9
135.1
133.0
132.2
131.9
129.8
128.8
128.6
128.3
127.4
123.5
117.9
114.5
109.8
77.3
77.0
76.7
55.5
50.1
46.5
42.3
32.5
31.8
29.2
27.3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3ai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F
N
N
OMe
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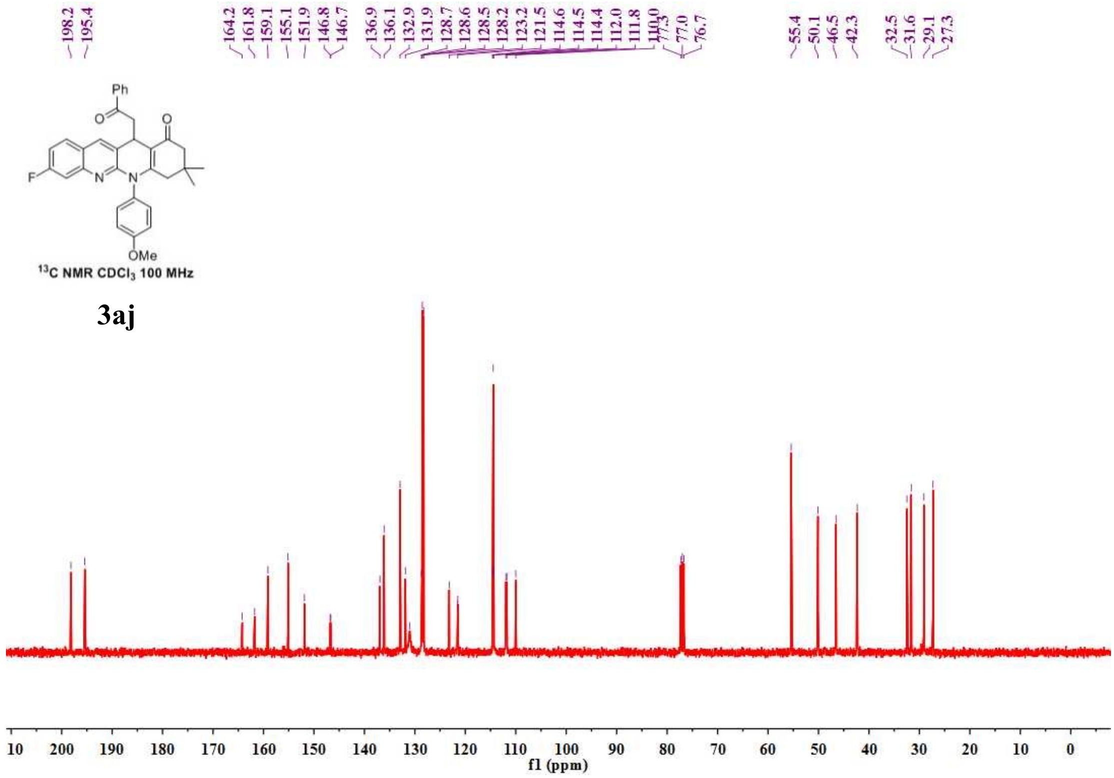
7.97
7.81
7.58
7.57
7.56
7.55
7.52
7.51
7.49
7.44
7.42
7.40
7.26
7.25
7.19
7.16
7.07
7.05
7.02
7.02
4.94
4.94
4.93
4.92
3.92
3.45
3.43
3.36
3.33
3.32
2.28
2.27
2.22
2.15
2.11
2.09
2.05
0.99
0.98
2.01
1.03
1.08
1.08
2.13
2.41
1.07
3.15
1.00
3.12
2.16
2.06
2.12
2.71
3.14
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3aj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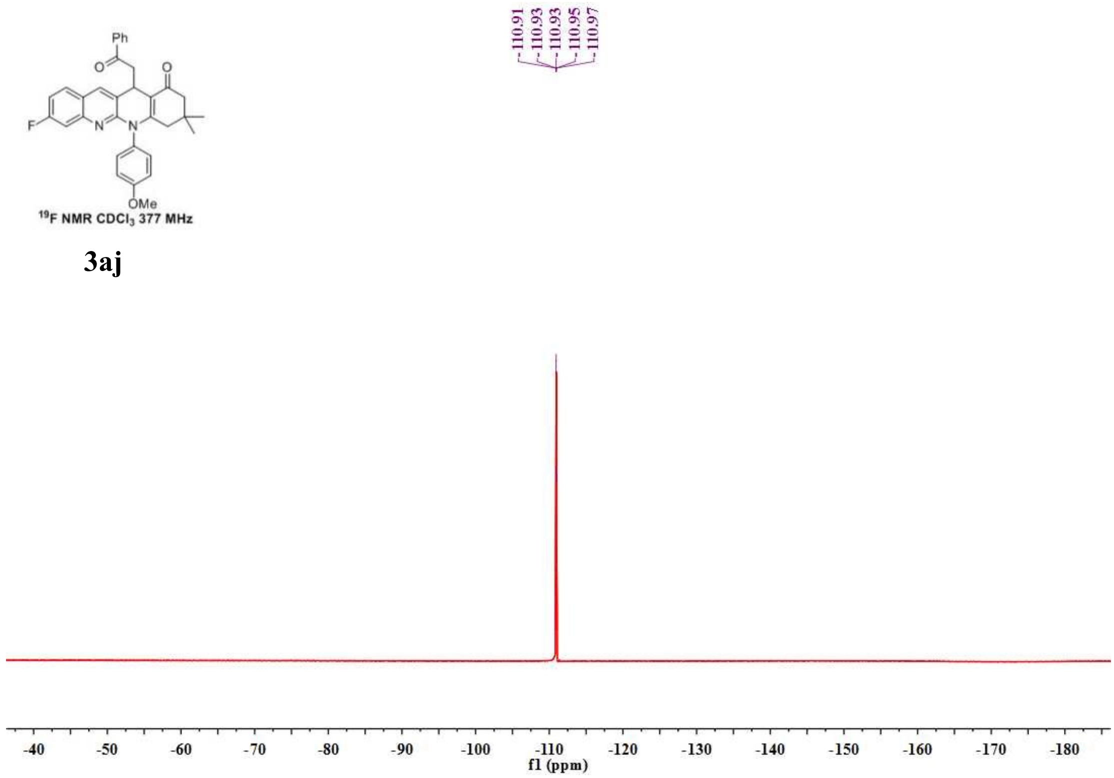
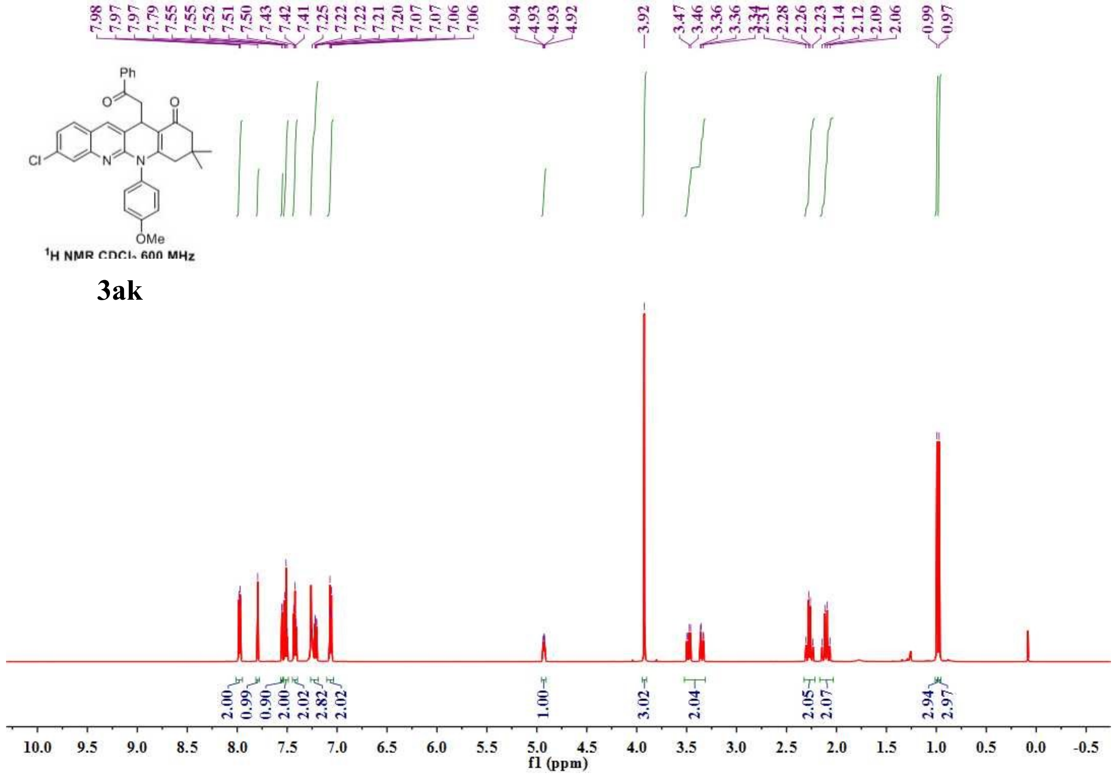
195.4
164.2
161.8
159.1
155.1
151.9
146.8
146.7
136.9
136.1
132.9
131.9
128.7
128.6
128.5
128.2
123.2
121.5
114.6
114.5
114.4
112.0
111.8
110.0
77.3
77.0
76.7
55.4
50.1
46.5
42.3
32.5
31.6
29.1
27.3
Ph
O
O
F
N
N
OMe
^{13}C NMR CDCl$_3$ 100 MHz
3aj
f1 (ppm)


110.91
110.93
110.93
110.95
110.97
Ph
O
O
F
N
N
OMe
^{19}F NMR CDCl$_3$ 377 MHz
3aj
f1 (ppm)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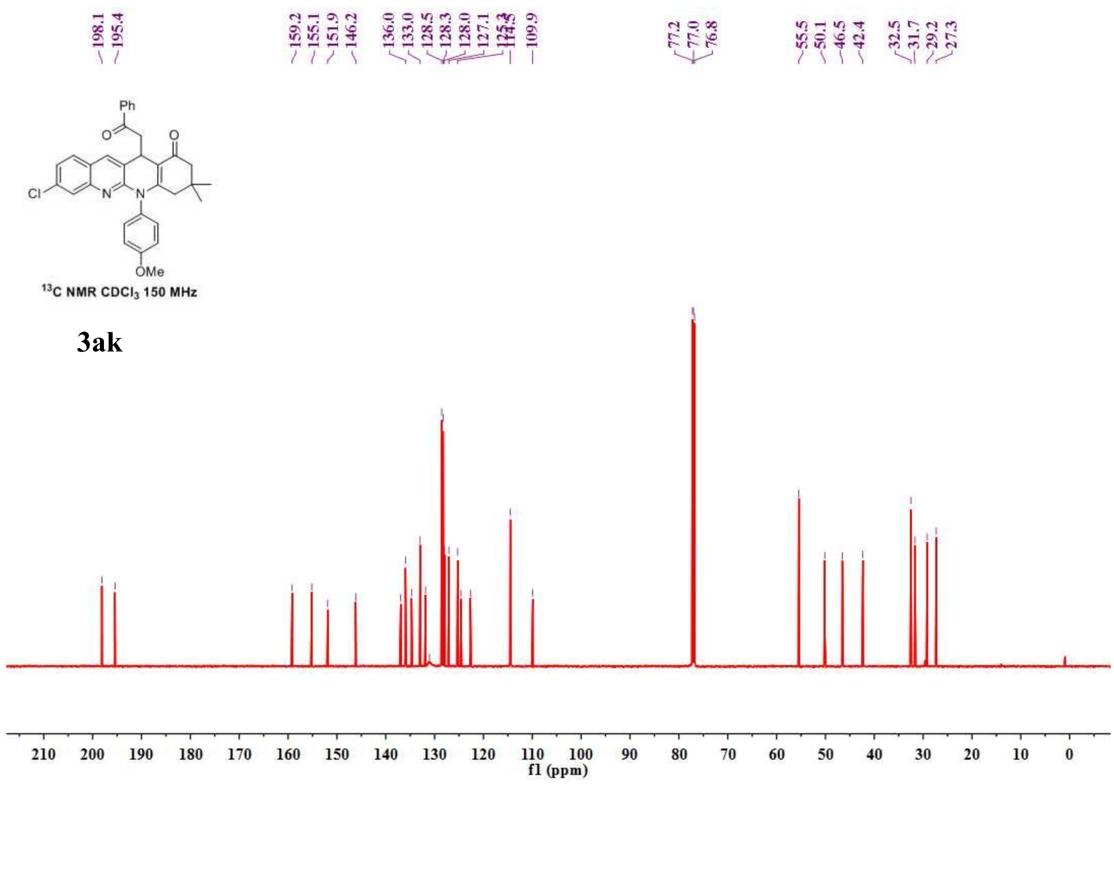
7.97
7.97
7.79
7.55
7.55
7.52
7.51
7.50
7.43
7.42
7.41
7.25
7.22
7.22
7.21
7.20
7.07
7.07
7.06
7.06
4.94
4.93
4.93
4.92
3.92
3.47
3.46
3.36
3.36
3.34
3.31
2.28
2.26
2.23
2.14
2.12
2.09
2.06
0.99
0.97
Ph
O
O
Cl
N
N
OMe
1H NMR CDCl3 600 MHz
2.00
0.99
0.90
2.00
2.02
2.82
2.02
1.00
3.02
2.04
2.05
2.07
2.94
2.97
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

3ak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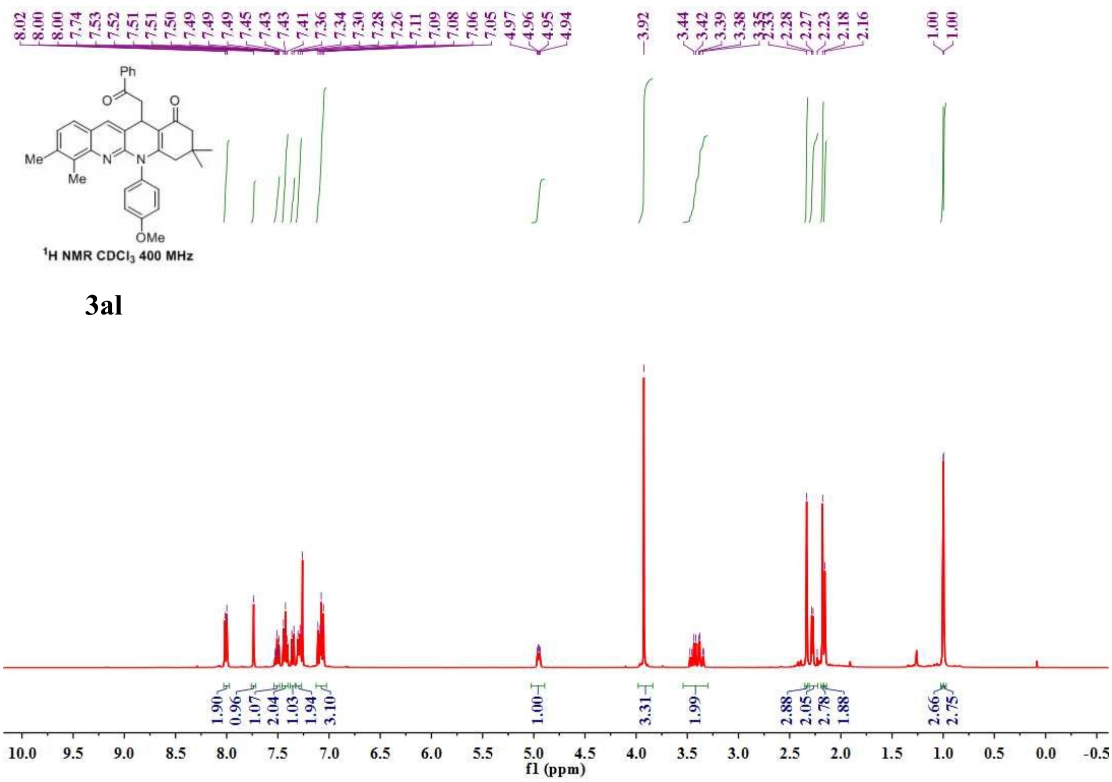
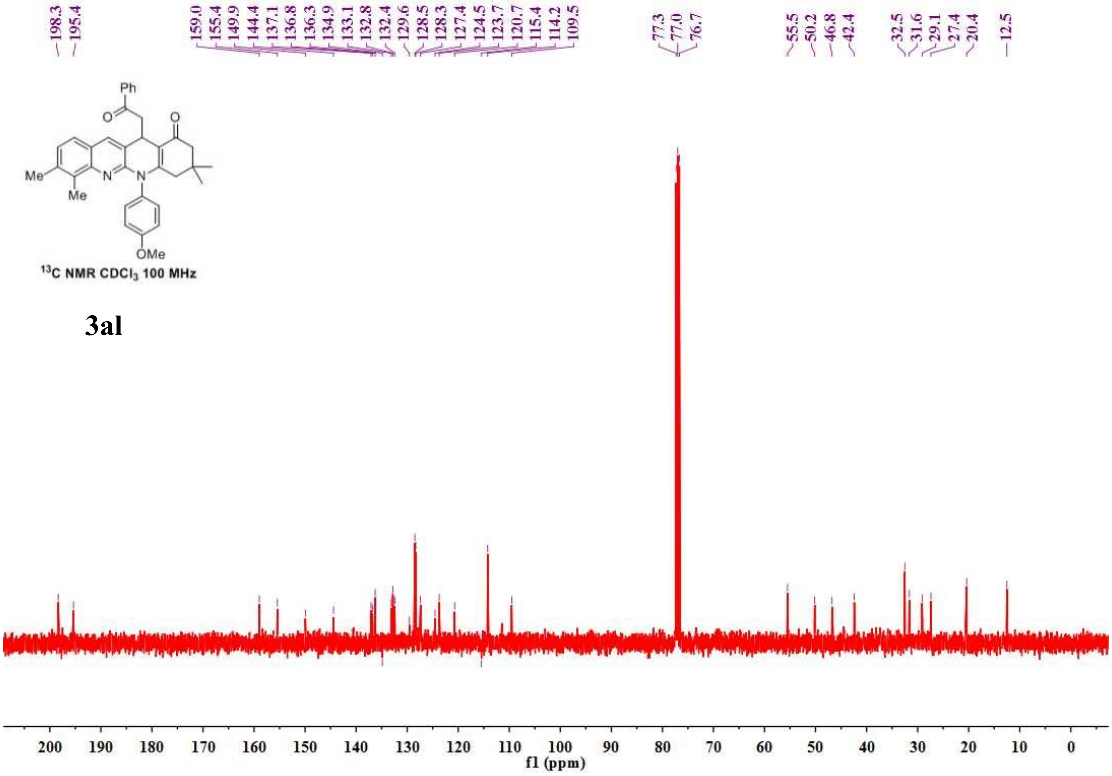
195.4
159.2
155.1
151.9
146.2
136.0
133.0
128.5
128.3
128.0
127.1
125.3
114.5
109.9
77.2
77.0
76.8
55.5
50.1
46.5
42.4
32.5
31.7
29.2
27.3
Ph
O
O
Cl
N
N
OMe
13C NMR CDCl3 150 MHz
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3ak



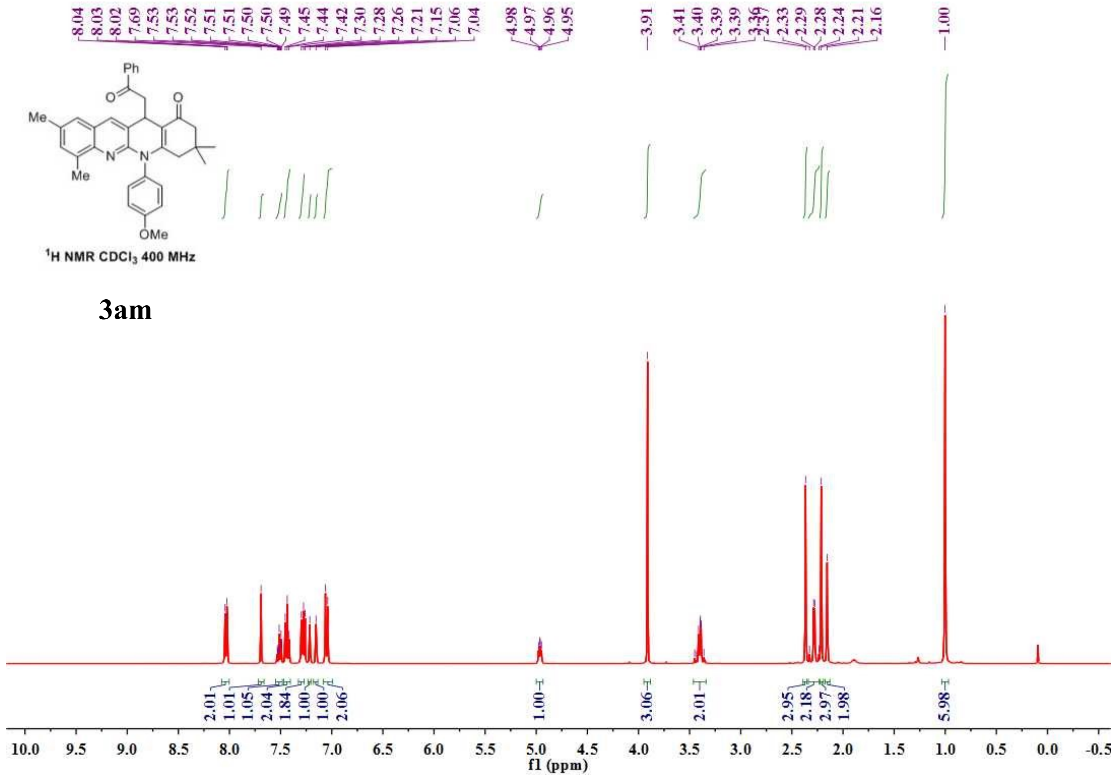
8.02 8.00 7.74 7.53 7.52 7.51 7.51 7.50 7.49 7.49 7.45 7.43 7.43 7.41 7.36 7.34 7.30 7.28 7.26 7.11 7.09 7.08 7.06 7.05 4.97 4.96 4.95 4.94 3.92 3.44 3.42 3.39 3.38 3.35 2.33 2.28 2.27 2.23 2.18 2.16 1.00 1.00
Ph
O
O
Me
Me
N
N
OMe
1H NMR CDCl3 400 MHz
1.90 0.96 1.07 2.04 1.03 1.94 3.10 1.00 3.31 1.99 2.88 2.05 2.78 1.88 2.66 2.75
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3al

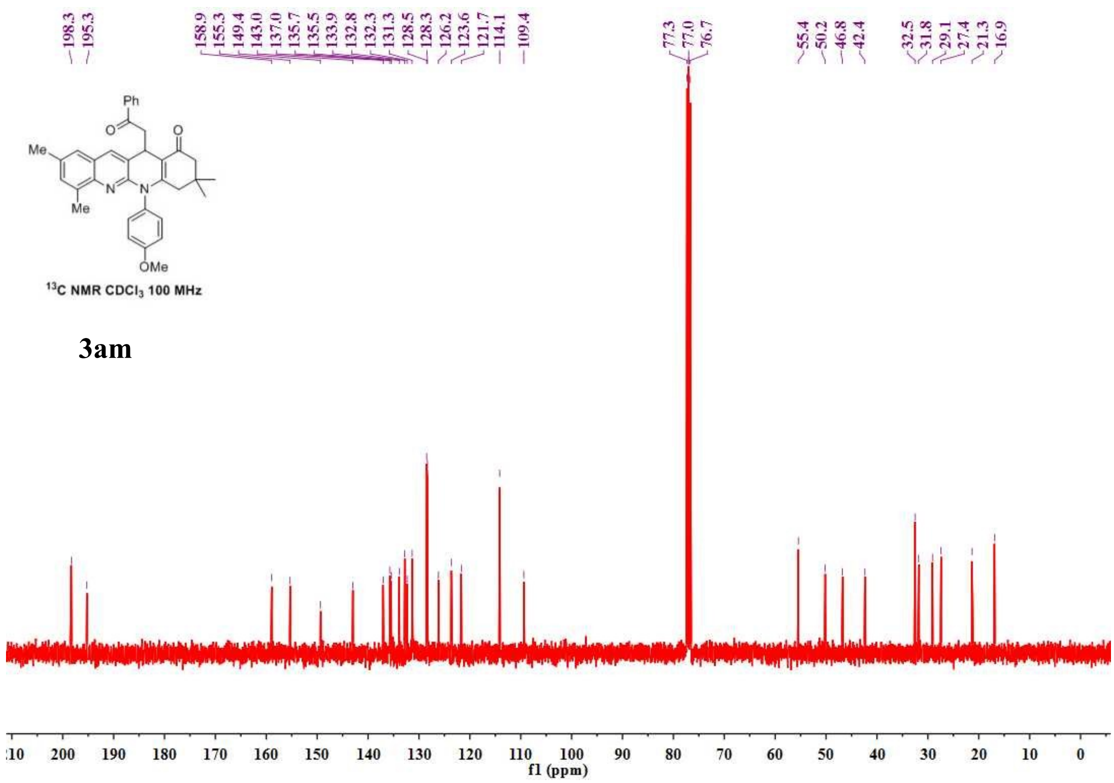


198.3 195.4 159.0 155.4 149.9 144.4 137.1 136.8 136.3 134.9 133.1 132.8 132.4 129.6 128.5 128.3 127.4 124.5 123.7 120.7 115.4 114.2 109.5 77.3 77.0 76.7 55.5 50.2 46.8 42.4 32.5 31.6 29.1 27.4 20.4 12.5
Ph
O
O
Me
Me
N
N
OMe
13C NMR CDCl3 100 MHz
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

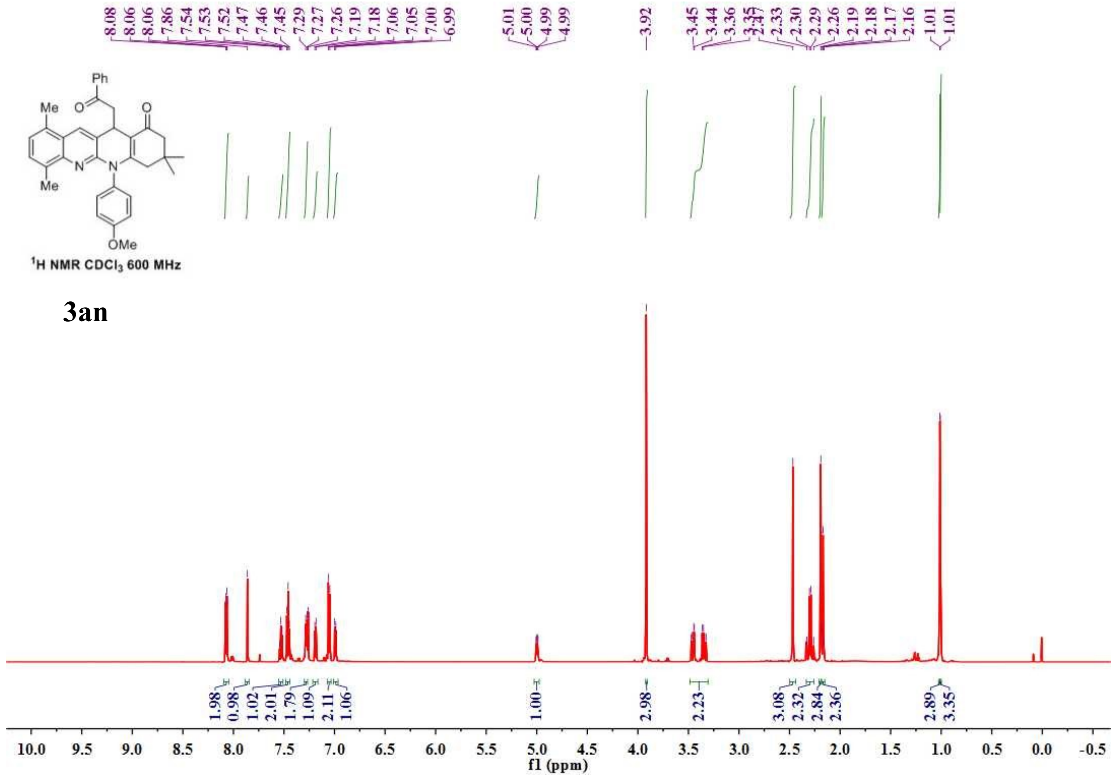
3al



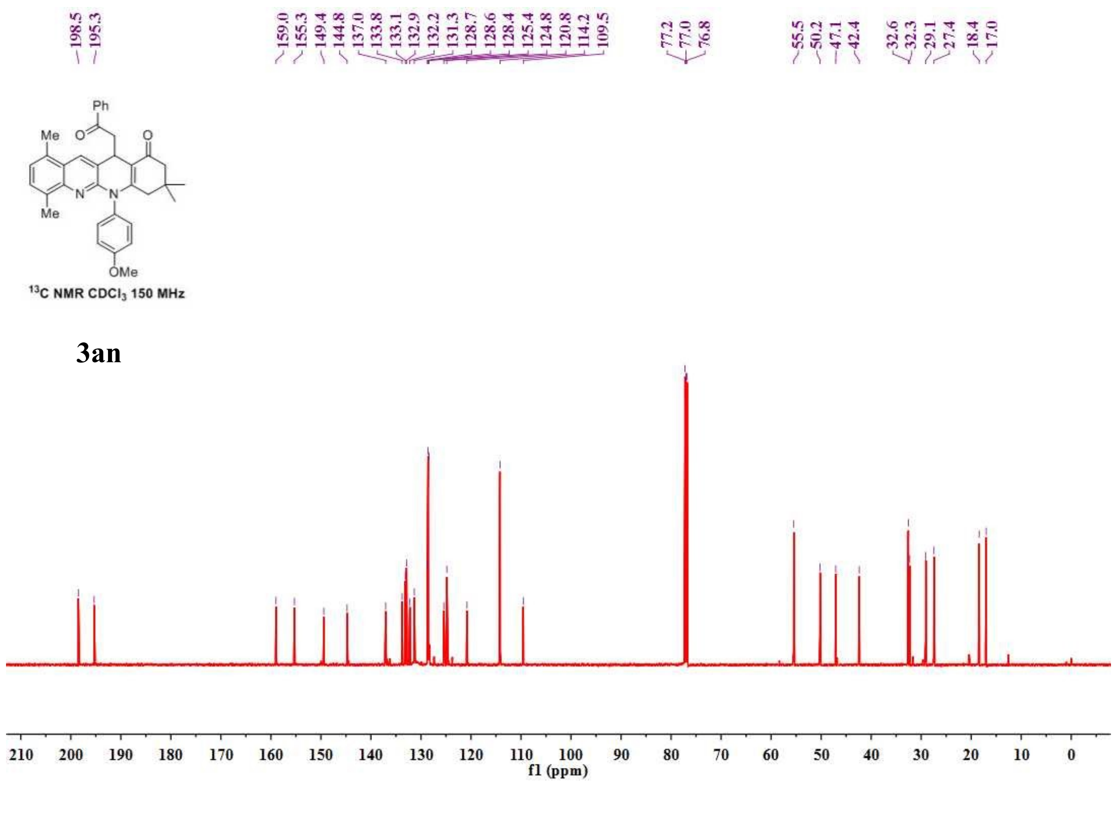
3am



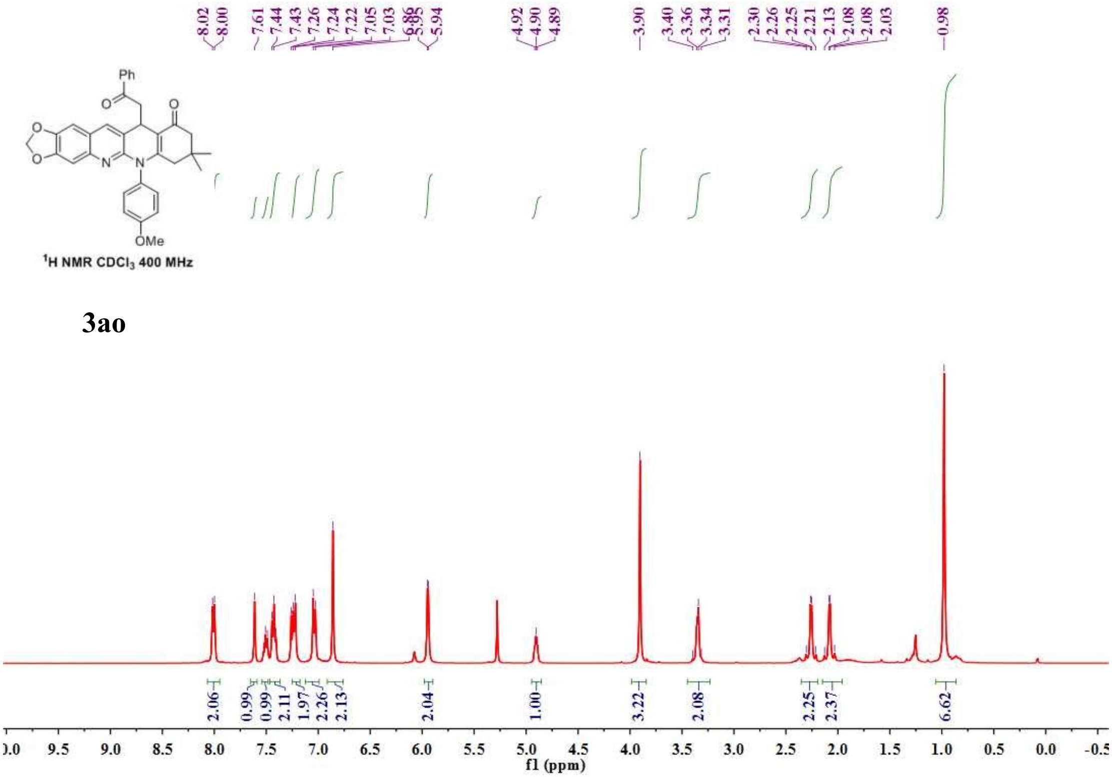
3am



¹H NMR CDCl₃ 600 MHz
3an
f1 (ppm)



¹³C NMR CDCl₃ 150 MHz
3an
f1 (ppm)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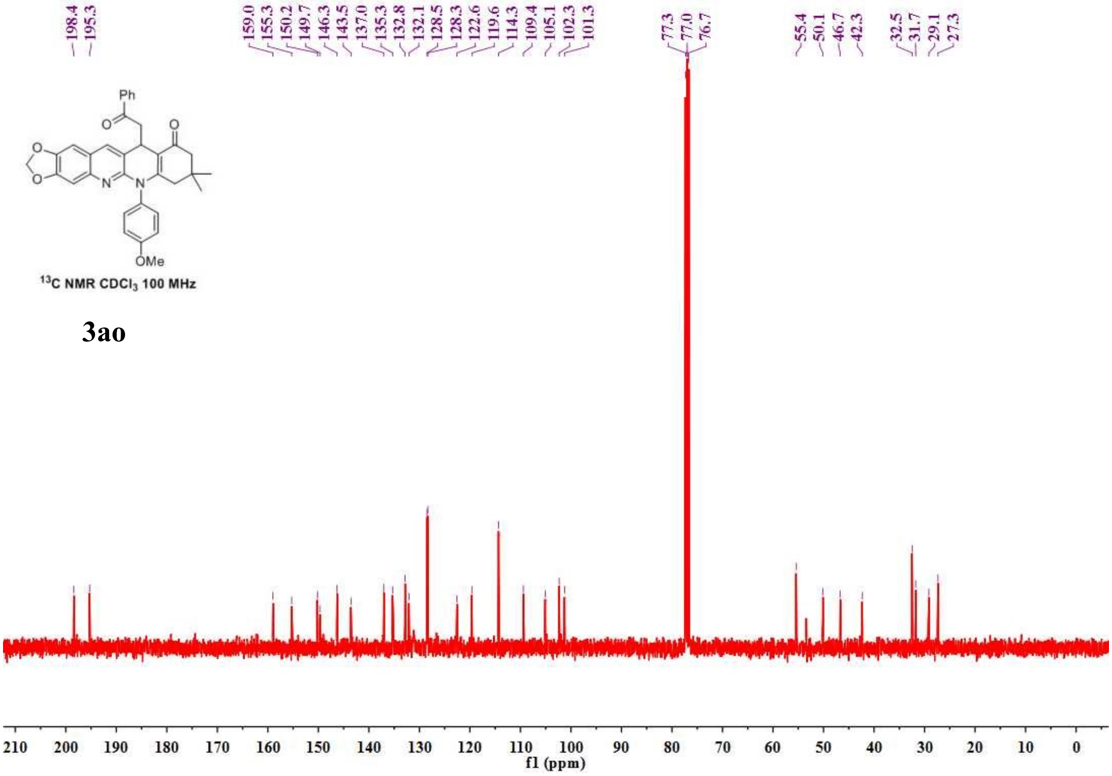
8.00
7.61
7.44
7.43
7.26
7.24
7.22
7.05
7.03
6.86
5.95
5.94
4.92
4.90
4.89
3.90
3.40
3.36
3.34
3.31
2.30
2.26
2.25
2.21
2.13
2.08
2.08
2.03
0.98
Ph
O
O
O
N
N
OMe
¹H NMR CDCl₃ 400 MHz
2.06
0.99
0.99
2.11
1.97
2.26
2.13
2.04
1.00
3.22
2.08
2.25
2.37
6.62
f1 (ppm)

3ao


198.4
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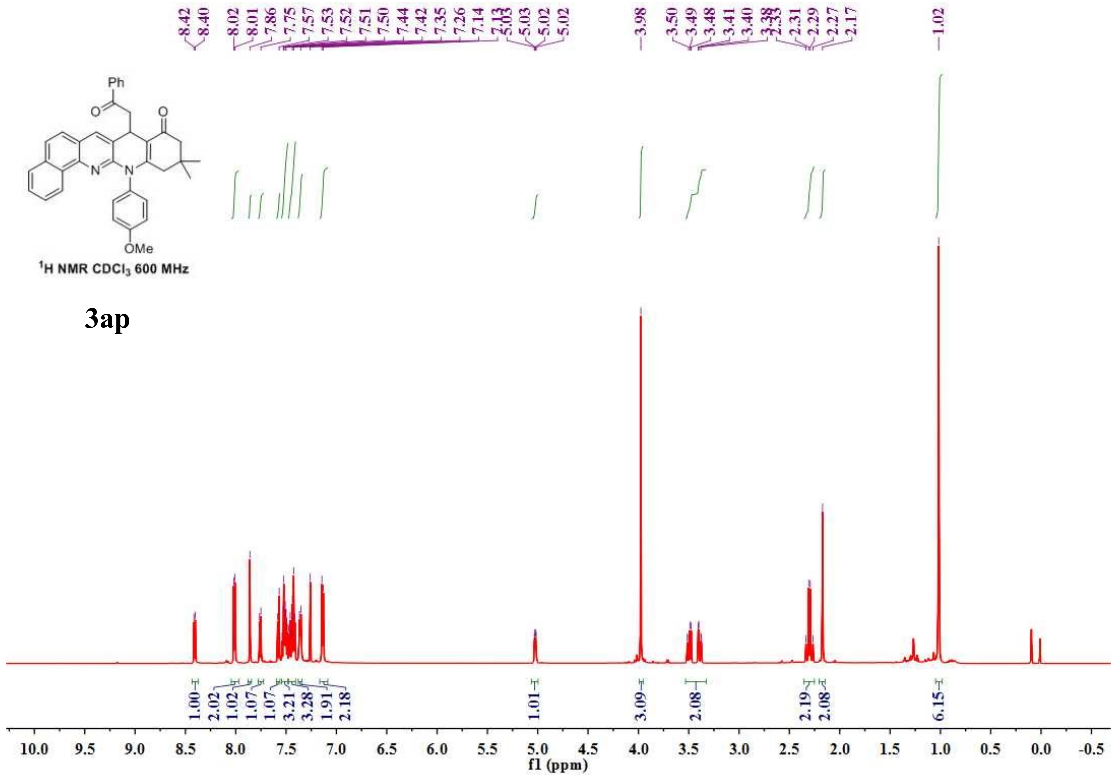
155.3
150.2
149.7
146.3
143.5
137.0
135.3
132.8
132.1
128.5
128.3
122.6
119.6
114.3
109.4
105.1
102.3
101.3
77.3
77.0
76.7
55.4
50.1
46.7
42.3
32.5
31.7
29.1
27.3
Ph
O
O
O
N
N
OMe
¹³C NMR CDCl₃ 100 MHz
f1 (ppm)

3ao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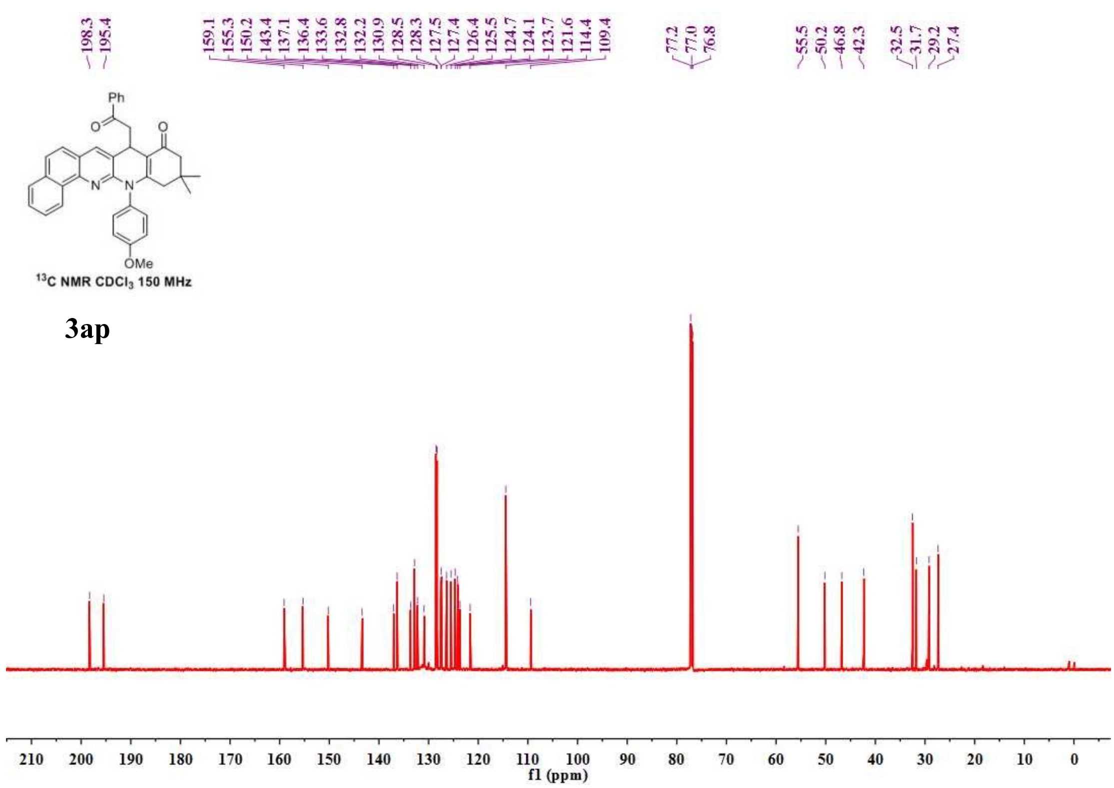
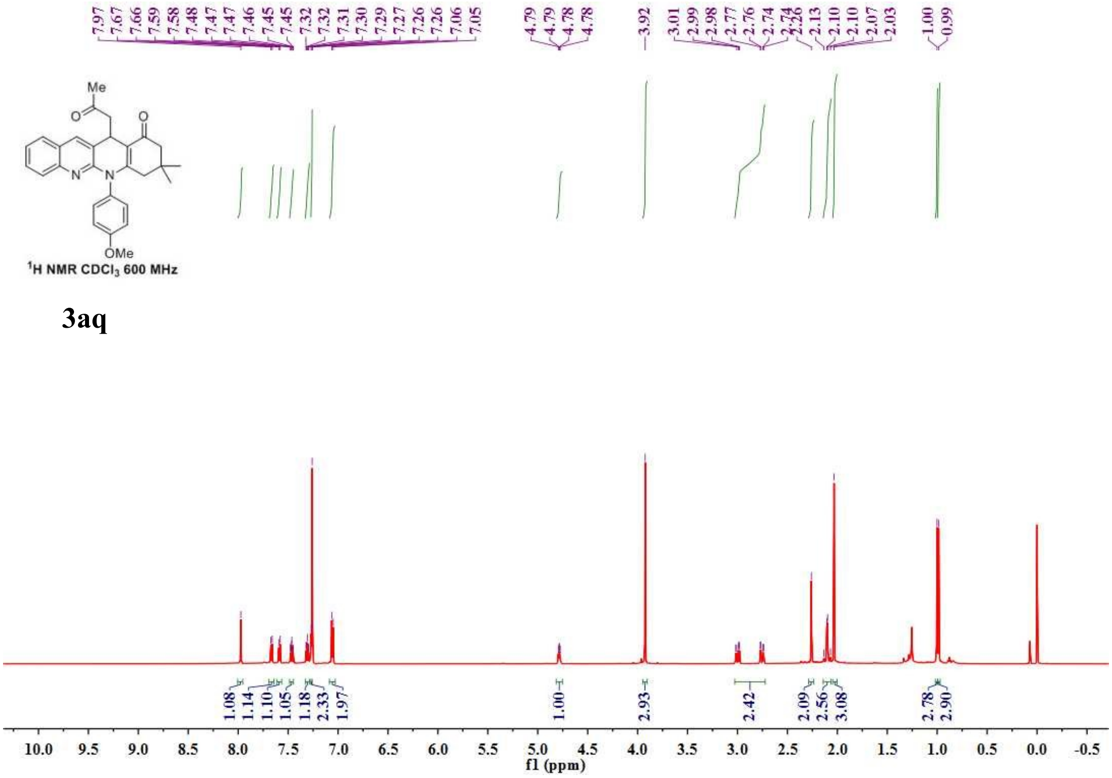
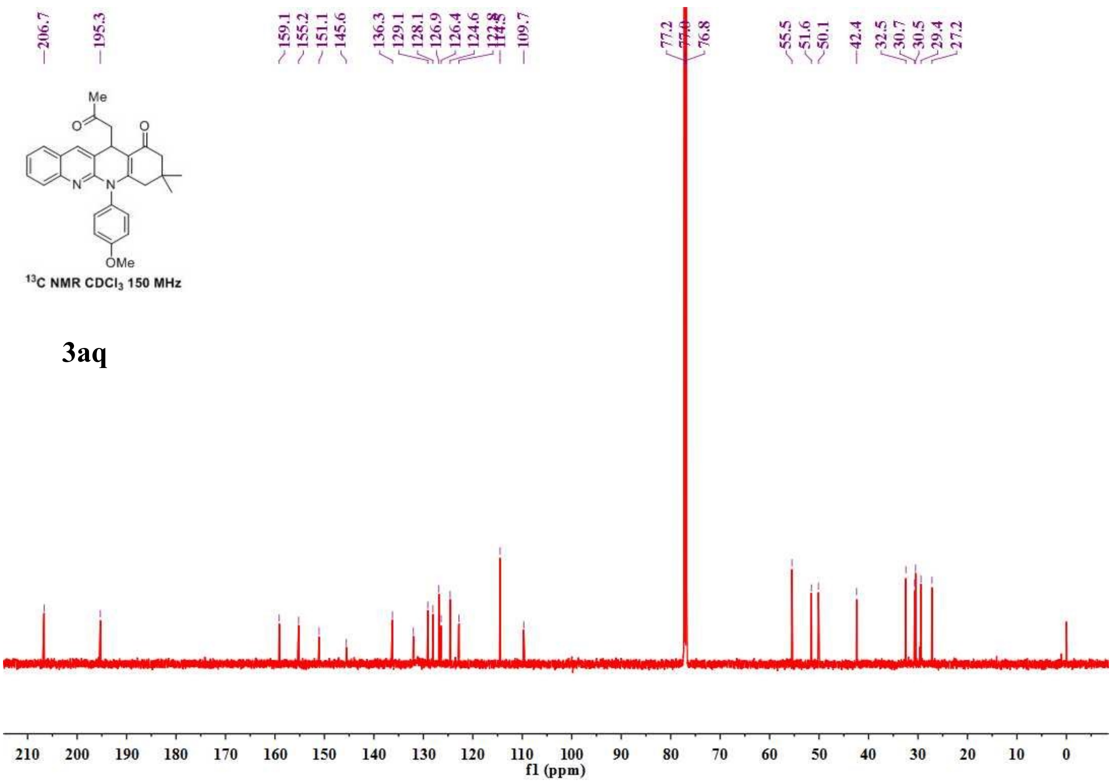
3.98
3.50 3.49 3.48 3.41 3.40 3.38 3.35 2.31 2.29 2.27 2.17
1.02
Ph
O
N
OMe
1H NMR CDCl3 600 MHz
3ap
1.00 2.02 1.02 1.07 1.07 3.21 3.28 1.91 2.18
1.01
3.09
2.08
2.19 2.08
6.15
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


198.3 195.4
159.1 155.3 150.2 143.4 137.1 136.4 133.6 132.8 132.2 130.9 128.5 128.3 127.5 127.4 126.4 125.5 124.7 124.1 123.7 121.6 114.4 109.4
77.2 77.0 76.8
55.5 50.2 46.8 42.3
32.5 31.7 29.2 27.4
Ph
O
N
OMe
13C NMR CDCl3 150 MHz
3ap
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



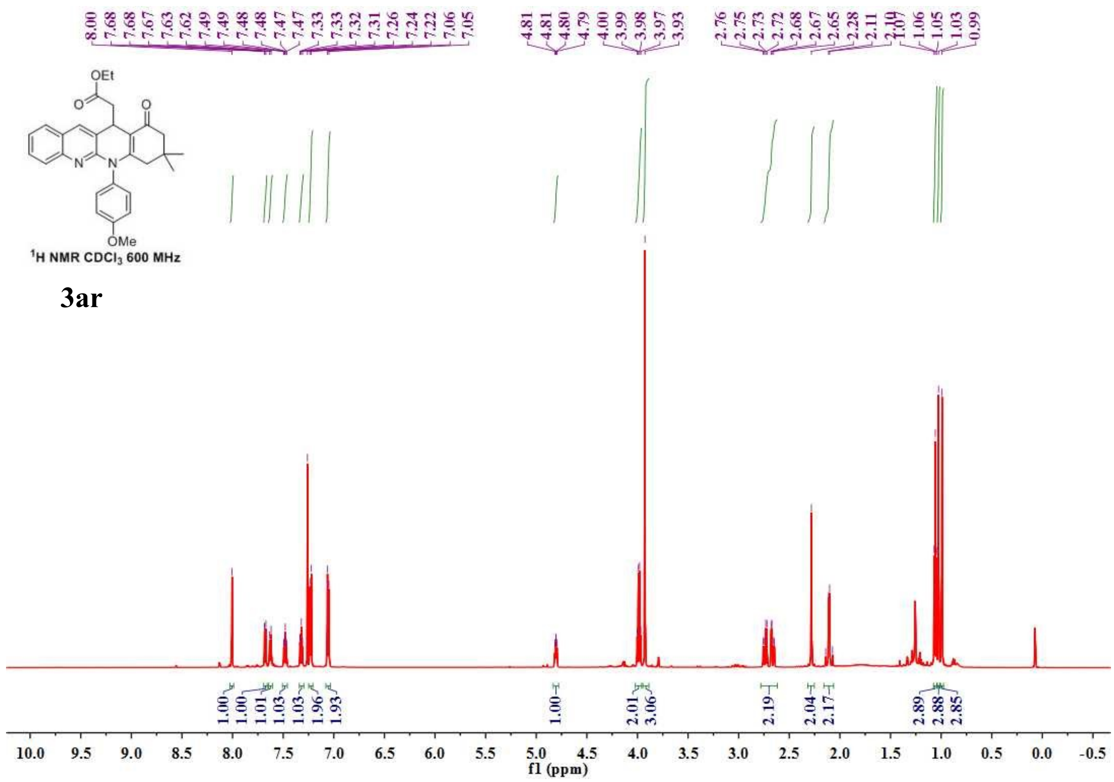
7.97 7.67 7.66 7.59 7.58 7.48 7.47 7.47 7.46 7.45 7.45 7.32 7.32 7.31 7.30 7.29 7.27 7.26 7.26 7.06 7.05
4.79 4.79 4.78 4.78
3.92
3.01 2.99 2.98 2.77 2.76 2.74 2.74 2.26 2.13 2.10 2.10 2.07 2.03
1.00 0.99
Me
O
O
N
N
OMe
1H NMR CDCl3 600 MHz
1.08 1.14 1.10 1.05 1.18 2.33 1.97
1.00
2.93
2.42
2.09 2.56 3.08
2.78 2.90
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3aq

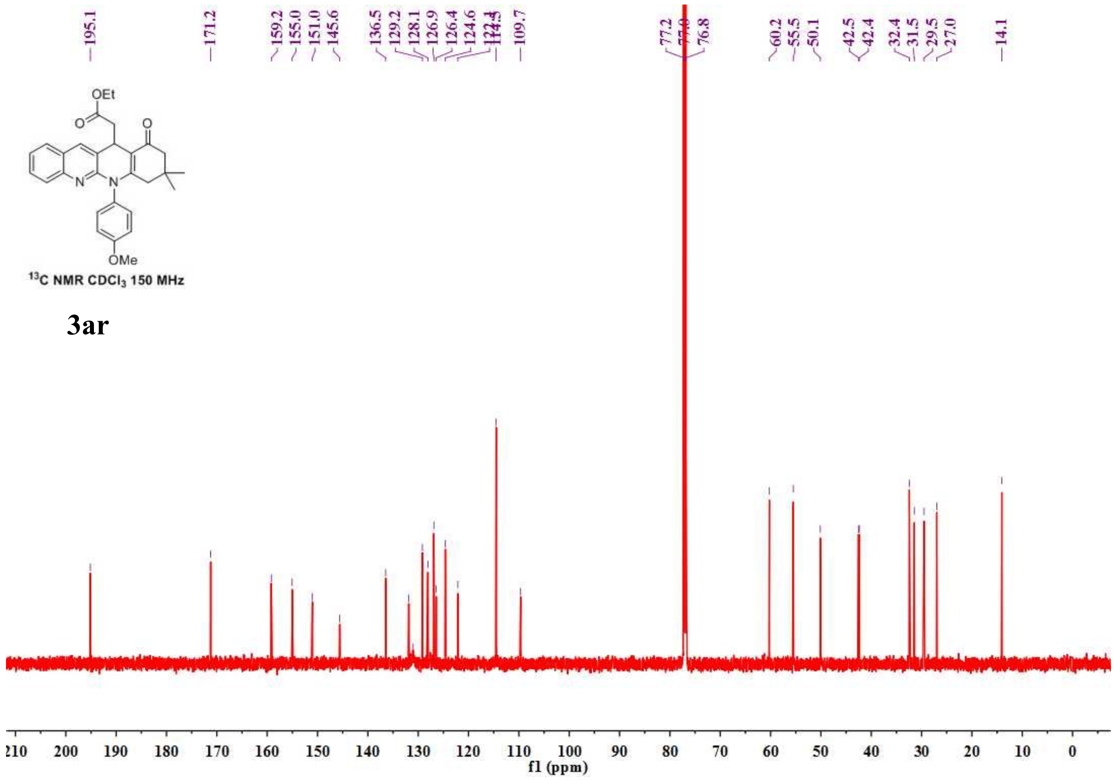


206.7
195.3
159.1 155.2 151.1 145.6
136.3 129.1 128.1 126.9 126.4 124.6
109.7
77.2 77.0 76.8
55.5 51.6 50.1
42.4
32.5 30.7 30.5 29.4 27.2
Me
O
O
N
N
OMe
13C NMR CDCl3 150 MHz
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

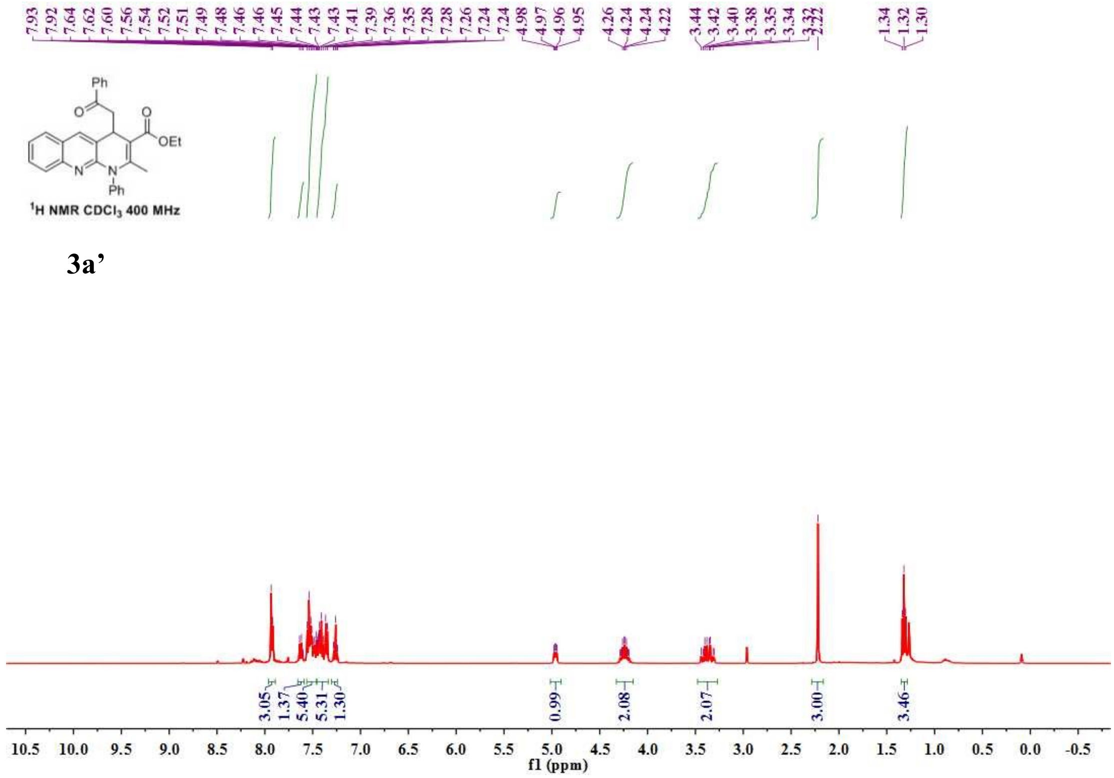
3aq



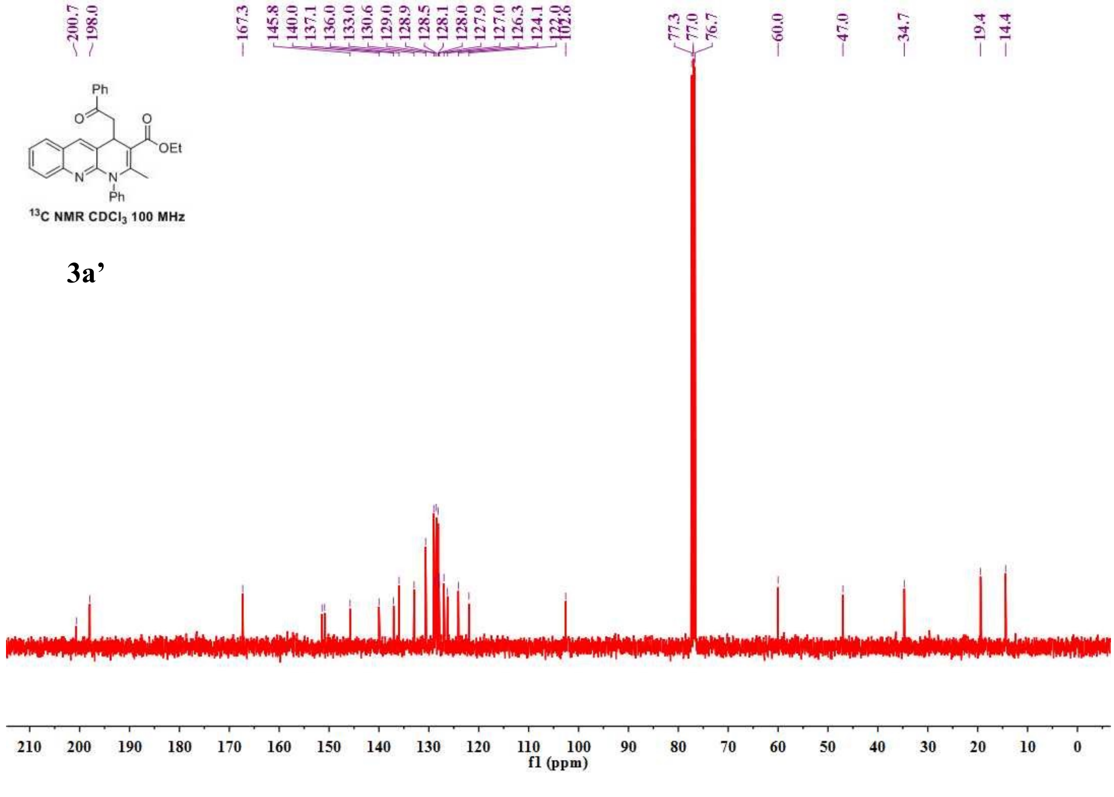
3ar



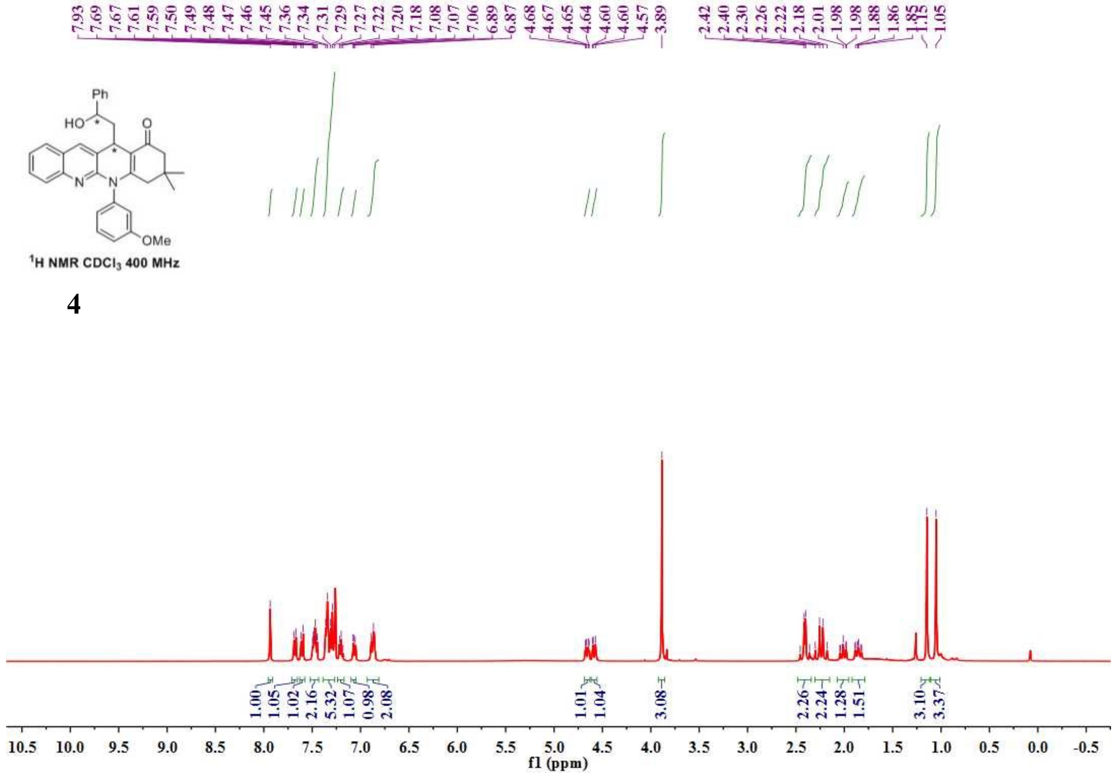
3ar


Ph
O
OEt
N
N
Ph
¹H NMR CDCl₃ 400 MHz
7.93 7.92 7.64 7.62 7.60 7.56 7.54 7.52 7.51 7.49 7.48 7.46 7.46 7.45 7.44 7.43 7.43 7.41 7.39 7.36 7.35 7.28 7.26 7.24 7.24 4.98 4.97 4.96 4.95 4.26 4.24 4.24 4.22 3.44 3.42 3.40 3.38 3.35 3.34 3.32 2.22 1.34 1.32 1.30
3.05 1.37 5.40 5.31 1.30 0.99 2.08 2.07 3.00 3.46
f1 (ppm)

3a’

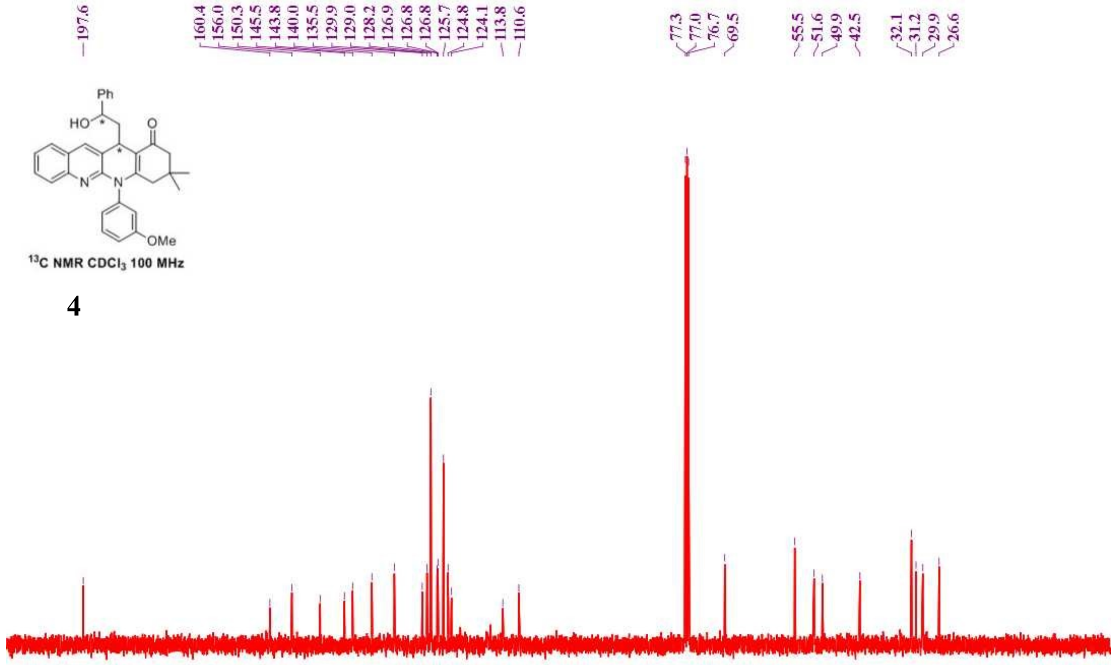

200.7 198.0 167.3 145.8 140.0 137.1 136.0 133.0 130.6 129.0 128.9 128.5 128.1 128.0 127.9 127.0 126.3 124.1 122.0 102.6 77.3 77.0 76.7 60.0 47.0 34.7 19.4 14.4
Ph
O
OEt
N
N
Ph
¹³C NMR CDCl₃ 100 MHz
f1 (ppm)

3a’



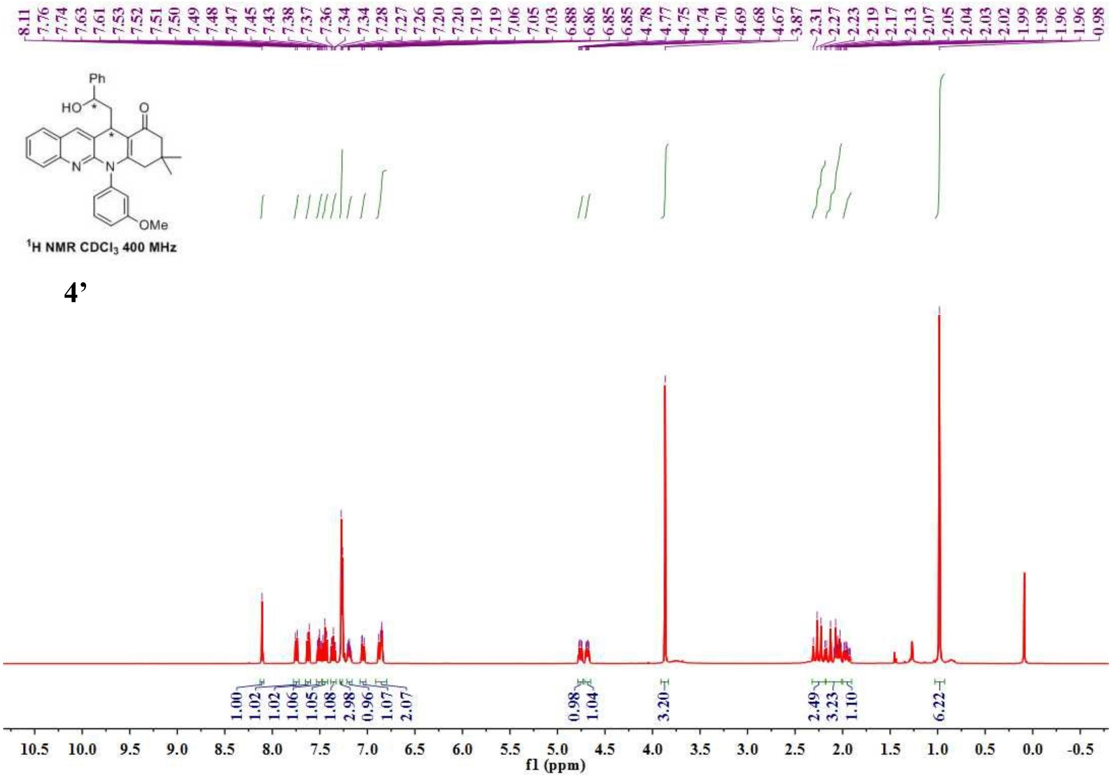
^{1}H NMR CDCl$_3$ 400 MHz

4

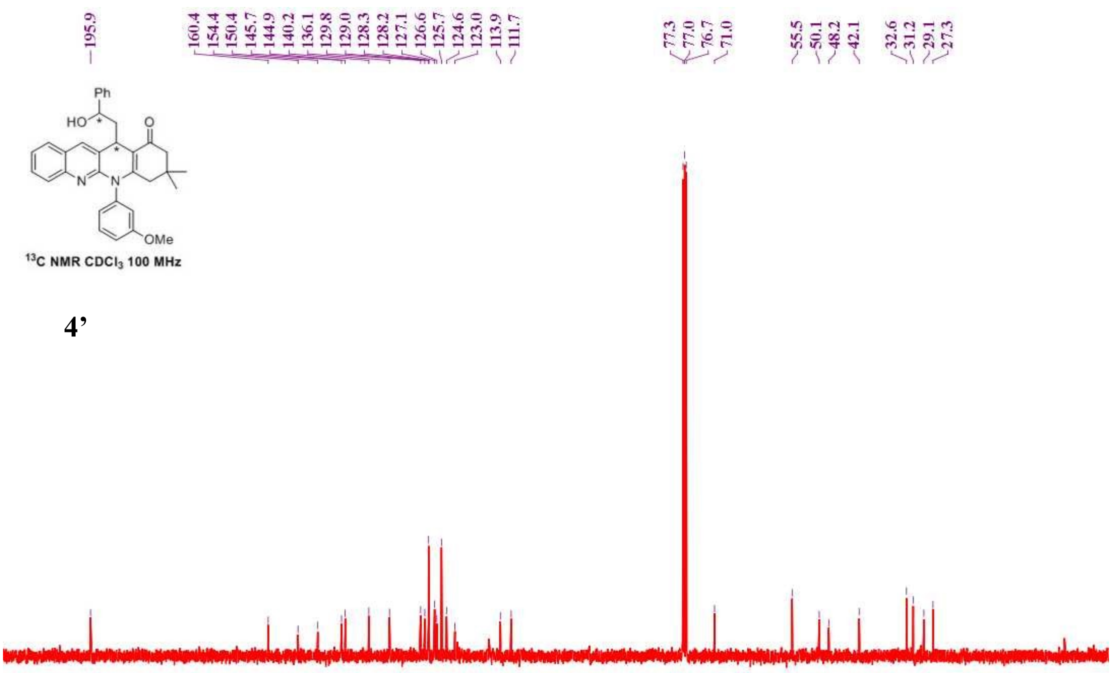


^{13}C NMR CDCl$_3$ 100 MHz

4



4’



4’